

AN APPLICATION OF DIOPHANTINE APPROXIMATION TO THE CONSTRUCTION OF RANK-1 LATTICE QUADRATURE RULES

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ABSTRACT. Lattice quadrature rules were introduced by Frolov (1977), Sloan (1985) and Sloan and Kachoyan (1987). They are quasi-Monte Carlo rules for the approximation of integrals over the unit cube in \mathbb{R}^s and are generalizations of ‘number-theoretic’ rules introduced by Korobov (1959) and Hlawka (1962)—themselves generalizations, in a sense, of rectangle rules for approximating one-dimensional integrals, and trapezoidal rules for periodic integrands.

Error bounds for rank-1 rules are known for a variety of classes of integrands. For periodic integrands with unit period in each variable, these bounds are conveniently characterized 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 nodes) then becomes that of finding rules with large values of ρ . This paper presents a new approach, based on the theory of simultaneous Diophantine approximation, which uses a generalized continued fraction algorithm to construct rank-1 rules of high order.

1. INTRODUCTION

Lattice rules for multiple integrals were introduced by Frolov [12], Sloan [37] and Sloan and Kachoyan [40]. These are quasi-Monte Carlo rules which are tuned to a particular class of functions and region of integration, namely, periodic functions over a hypercube. Their range of applicability may be extended by a variety of techniques (see, for example, [2], [15], [33], [34], [48]). Lattice rules generalize an earlier type of quasi-Monte Carlo method, the so-called ‘method of good lattice points’, introduced by Korobov [19], [20], Bakhvalov [1] and Hlawka [14]. The abscissa set is determined, in the method of good lattice points, by the choice of one fixed rational vector, say \mathbf{g}/N , where $\gcd(g_1, \dots, g_s, N) = 1$, called the *generator* of the rule. The number N of nodes is called the *order* of the rule. The accuracy achievable by the integration rule depends directly on the particular combination of \mathbf{g} and N chosen (see, for example, [14], [29], [47]). Lattice rules generalize this method by allowing the choice of more than a single generator. Surveys of the

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theory of lattice rules have recently been given by Niederreiter [30], Sloan [38] and Sloan and Joe [39].

An *integration lattice* in \mathbb{R}^s is a discrete additive subgroup L of \mathbb{R}^s which contains \mathbb{Z}^s . The points of an integration lattice L are rational vectors. An s -dimensional lattice rule is an equal-weight quadrature rule Q_L defined on the half-open unit cube

$$U^s = \underbrace{[0, 1) \times [0, 1) \times \cdots \times [0, 1)}_{s \text{ factors}}.$$

It may be expressed in the form

$$(1.1) \quad Q_L(f) = \frac{1}{N} \sum_{\mathbf{x} \in A(Q_L)} f(\mathbf{x}),$$

where $A(Q_L) = L \cap U^s$ is the set of quadrature points and N is the order of the rule. Sloan and Lyness [41] observed that, for any lattice rule, $A(Q_L)$ is a finite Abelian group under addition modulo \mathbb{Z}^s and consequently that Q_L can be expressed in a nonrepetitive canonical form:

$$(1.2) \quad Q_L(f) = \frac{1}{N} \sum_{j_1=0}^{n_1-1} \cdots \sum_{j_m=0}^{n_m-1} f\left(\left\{\sum_{i=1}^m \frac{j_i}{n_i} \mathbf{g}_i\right\}\right),$$

where $m \leq s$, the vectors $\mathbf{g}_1, \dots, \mathbf{g}_m$ are fixed integral vectors, $N = \prod_{i=1}^m n_i$, and $n_{i+1} \mid n_i$ for $i = 1, \dots, m-1$, with $n_m > 1$. The braces in (1.2) 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 .

In (1.2) the parameters m, n_1, \dots, n_m are uniquely determined for a given rule, and are called the *rank* (m) and *invariants* (n_1, \dots, n_m) of the rule. The vectors \mathbf{g}_i/n_i are not uniquely determined—they form a *generator set* for $A(Q_L)$. Sloan and Lyness [41] also pointed out that lattice rules may be classified according to their ranks and invariants. Methods for determining the rank, invariants and a canonical form of a lattice rule have been described briefly by Worley [46] and in more detail by Langtry [23] and Lyness and Keast [24].

How well a particular rule approximates the integral

$$I(f) = \int_{U^s} f(\mathbf{x}) dV,$$

where dV is the volume element in U^s , depends upon the underlying choice of $A(Q_L)$, and thus upon the generator set. Bounds on the absolute approximation error $|I(f) - Q_L(f)|$ are known for a variety of classes of rules and a variety of classes of functions (see, for example, [9], [10], [30], [31], [32], [43]). Intuitively, a rule is 'good' if this bound is small compared with the average error of rules of the same order.

For functions f which are 1-periodic in each variable the rule defined by (1.1) is the s -dimensional analogue of the one-dimensional trapezoidal rule, which is known to perform very well for periodic functions. In this paper we consider the determination of good s -dimensional rank-1 lattice rules for 1-periodic continuous functions with absolutely and uniformly convergent Fourier series. Such functions may be classified according to the bounds satisfied by their Fourier coefficients.

Define

$$(1.3) \quad r(\mathbf{h}) = \prod_{j=1}^s \max\{1, |h_j|\}$$

for $\mathbf{h} \in \mathbb{Z}^s$, and denote by $\hat{f}(\mathbf{h})$ the Fourier coefficient at \mathbf{h} of $f : \mathbb{R}^s \rightarrow \mathbb{R}$, that is,

$$\hat{f}(\mathbf{h}) = \int_{U^s} f(\mathbf{x}) e^{-2\pi i \mathbf{h} \cdot \mathbf{x}} dV,$$

where i denotes the usual imaginary unit. For $c > 0$ and $\alpha, s > 1$, let

$$(1.4) \quad E_s^\alpha(c) = \left\{ f : |\hat{f}(\mathbf{h})| \leq \frac{c}{[r(\mathbf{h})]^\alpha}, \mathbf{h} \in \mathbb{Z}^s - \{\mathbf{0}\} \right\}.$$

Then for $f \in E_s^\alpha(c)$ it is known that

$$|Q_L(f) - I(f)| \leq c \sum_{\mathbf{h} \in L^\perp - \{\mathbf{0}\}} \frac{1}{[r(\mathbf{h})]^\alpha},$$

where L is generated by $\{\mathbf{g}_1/n_1, \dots, \mathbf{g}_m/n_m\} \cup \mathbb{Z}^s$ and $L^\perp = \{\mathbf{h} \in \mathbb{Z}^s : \forall \mathbf{x} \in L, \mathbf{x} \cdot \mathbf{h} \in \mathbb{Z}\}$. The integer lattice L^\perp is called the *dual* of L .

For $f \in E_s^\alpha(c)$, three quantities used as indicators of the quality of a rule Q_L are: the *figure of merit* ρ defined by

$$\rho(L) = \min\{r(\mathbf{h}) : \mathbf{h} \in L^\perp - \{\mathbf{0}\}\},$$

the *Zaremba index*

$$(1.5) \quad z_s = \rho \frac{(\log N)^{s-2}}{N},$$

and, for $\alpha > 1$, the error

$$(1.6) \quad P_\alpha = \sum_{\mathbf{h} \in L^\perp - \{\mathbf{0}\}} \frac{1}{r(\mathbf{h})^\alpha}$$

for the ‘worst’ function in the class $E_s^\alpha(1)$, incurred by using $Q_L(f)$ as an approximation to the required integral. For a discussion of the use of ρ and P_α see [30], [39] and for a discussion of z_s see [25], [26], [27].

For the class $E_s^\alpha(c)$ we may characterize as good those lattices which have large values of ρ relative to N (and hence large values of z_s), or small values of P_α . There have been two approaches used to find good rank-1 rules:

- (a) nonexhaustive and exhaustive searches of various classes of generators (e.g. [3], [13], [17], [28], [35]), and
- (b) construction of approximations to integral bases of algebraic number fields, or other irrational vectors (e.g. [15], [49]).

The rank-1 rules obtained by exhaustive searches have been of relatively low order, owing to the computational complexity of the search procedures used and the fact that this complexity increases rapidly with both dimension and order. Those obtained by nonexhaustive searches or by the constructions of Hua and Wang [15] have values of z_s much less than the best possible, as is evident from comparison with the numerical results presented in §6. The approach used by Zinterhof [49] appears to yield values of P_2 which are usually (not always) slightly inferior to those given in the tables of Maisonneuve [28] and Hua and Wang [15].

More recently, various constructions and searches of higher-rank rules have been carried out. As in the rank-1 case, the constructions that have been suggested (e.g. Worley [46]) have produced results that are generally much less satisfactory than those of the search procedures. Of particular interest are the searches of Sloan and Walsh [42], Lyness and Sørøvik [25], [26] and [27], and especially Disney and Sloan [11] which, as well as providing some very good rules, serve as a benchmark against which other approaches may be judged. In this paper we consider the class of rank-1 rules, originally introduced by Korobov [19], [20] and Hlawka [14], from the perspective of Diophantine approximation theory. For this class of rules there is theoretical (for $s = 2$, see [47]) and numerical (for $s > 2$) evidence which suggests that the majority of good rules may be generated by lattice points \mathbf{g} having one coordinate with value 1. Such rules are called *simple*. In the two-dimensional case Bakhvalov [1] and Zaremba [47] identified sequences of simple rules for which the values of $z_2 = \rho/N$ are best possible, in the sense that every rule with $N \geq 5$ in these sequences has a value of ρ exceeding that of any rule with the same number of points, or fewer, which is not a member of one of these sequences. In particular, the sequences are defined by

$$(1.7a) \quad \mathbf{g}_k = (1, F_{k-1}), \quad N_k = F_k, \quad \rho_k = F_{k-2},$$

$$(1.7b) \quad \mathbf{g}_k = (1, 2F_{k-1}), \quad N_k = 2F_k, \quad \rho_k = 2F_{k-2},$$

for $k \geq 3$, where $\{F_k\}$ is the Fibonacci sequence $1, 1, 2, 3, 5, \dots$.

The identification of the sequences of rules given by (1.7a) and (1.7b) as being the ‘best’, in the sense described above, relies on the machinery of continued fractions and its role in Diophantine approximation theory. In effect, for $s = 2$ the principal convergents of one of the worst approximable (in a sense which is made explicit in §4) irrational numbers produce the best possible rank-1 lattice rules. No analogous ‘best possible’ constructions in higher dimensions appear to be known. However, what appear to be ‘good’ constructions may be obtained by generalizing to higher dimensions aspects of the approach used by Zaremba [47] in dimension $s = 2$. In particular, we suggest that good choices of generators may be found amongst those vectors $(1, g_2, \dots, g_s)/N$ such that $(g_2, \dots, g_s)/N$ is not well approximated by rational vectors of lower denominator. Section 2 provides motivation for this suggestion from the two-dimensional case. In §3 a connection is established between generators for higher-dimensional rank-1 rules which are good with respect to ρ , and rational vectors \mathbf{v} which are badly approximated by rational vectors of lower denominator. It is then shown that the best approximating rational vectors to such vectors \mathbf{v} have denominators which are not widely separated. In §4 it is shown that sequences of such vectors \mathbf{v} may be found amongst approximations to certain badly approximable irrational vectors, via results of Lagarias [22]. More generally, similar, although weaker, results are obtained for rational vectors \mathbf{v} which are good approximations (in the sense of Definition 4.3), but not necessarily best approximations, to these irrational vectors.

Little appears to be known about fast methods for constructing best approximations to a given \mathbf{v} , for dimension $t > 2$. However, in practice the multidimensional continued fraction algorithms of Szekeres [44] and Brentjes [4] appear to construct good rational approximations for given \mathbf{v} . In §5 it is shown that the Szekeres algorithm may be adapted to produce a convergent sequence of rational vectors whose successive denominators grow slowly. In §6 we provide numerical evidence that the adapted algorithms can be used to produce good rank-1 lattice rules of high order.

Notation. It is assumed in the following that $N > 1$, s is an integer greater than or equal to 2, that $t = s - 1$, that \mathbf{g} has the form $\mathbf{g} = (1, g_2, \dots, g_s) \in \mathbb{Z}^s$ where $g_j > 0$, and that $\hat{\mathbf{g}} = (g_2, \dots, g_s)$. It is also assumed that v is a positive real number and that $\mathbf{v} = (v_1, \dots, v_t) \in \mathbb{R}^t$. We shall use the notation $\rho = \rho(L)$, where $L = L(\mathbf{g}/N)$ is the integration lattice generated by $\mathbb{Z}^s \cup \{\mathbf{g}/N\}$. The continued fraction expansion of a positive real number, say x , is denoted by

$$x = [a_0; a_1, a_2, \dots, a_k, \dots]$$

with the obvious modification for a terminating continued fraction in the case that x is rational: $x = [a_0; a_1, a_2, \dots, a_k]$. Clearly, in this case it may always be assumed that $a_k > 1$ when $k \geq 1$, since $[a_0; a_1, \dots, a_k, 1] = [a_0; a_1, \dots, a_k + 1]$. Frequent reference will be made to the theory of simple continued fractions. A suitable introduction to this theory may be found in Khinchin [18].

2. MOTIVATION IN THE TWO-DIMENSIONAL CASE

Let Q_L be a rank-1 simple rule in two dimensions generated by a vector of the form \mathbf{g}/N , where $\mathbf{g} = (1, g_2)$, $\gcd(g_2, N) = 1$ and $g_2/N = [0; a_1, a_2, \dots, a_k]$. Zaremba [47, Propositions 2.1 and 2.2] showed that the value of ρ is subject to the bounds

$$(2.1) \quad \frac{N}{M+2} \leq \rho \leq \frac{N}{M},$$

where $M = \max_{i \in \{1, \dots, k\}}(a_i)$. In particular, the proof of the lower bound relies on showing that ρ is achieved at a vector $\mathbf{h} \in L^\perp$ for which $|h_2| < N$. Zaremba then showed that, by definition of L^\perp , there exists an integer λ satisfying $h_1 + g_2 h_2 = \lambda N$ such that, letting $\bar{h}_i = \max(1, |h_i|)$,

$$\frac{\rho}{N} = \frac{\bar{h}_1}{N} \bar{h}_2 \geq \left| \frac{g_2}{N} h_2 - \lambda \right| \bar{h}_2 \geq \frac{\bar{h}_2}{(M+2)\bar{h}_2},$$

where the final inequality follows from the application of a well-known approximation result from the theory of continued fractions (see [18, Theorem 13]). For more details, the reader is referred to [47]. The bounds expressed in (2.1) characterize the value of ρ in terms of the continued fraction for g_2/N and suggest choices of generators which may yield desirable values of ρ . However, the author is not aware of any higher-dimensional generalization of the continued fraction algorithm for which an analogous approximation theorem is known, nor does it appear that Zaremba's results have hitherto been generalized to higher dimensions. In the remainder of this section we show that the choices of generator \mathbf{g}/N suggested by the bounds in (2.1) can also be characterized by the related properties that:

- (i) g_2/N is badly approximated by rationals of lower denominator, in the sense described later in this section, and
- (ii) the denominators of best rational approximations to g_2/N are not widely separated.

The following facts will be required. Let v be a positive real number. Then,

- (a) the rational p/q , where p, q are coprime, is a best approximation of v if:
 - (i) $|qv - p| = \min_{p' \in \mathbb{Z}} |qv - p'|$, and
 - (ii) $|q'v - p'| > |qv - p|$ for all $0 < q' < q$ and all $p' \in \mathbb{Z}$,

- (b) the principal convergents of the continued fraction for v are nonnegative and, except possibly for the first one, are precisely the best approximations of v in order of increasing denominator, and
- (c) the numerators and denominators of the principal convergents for $v = [a_0; a_1, \dots]$ satisfy the following recurrence relations. Define $p_{-1} = 1$ and $q_{-1} = 0$. Then $p_0 = a_0$, $q_0 = 1$ and, for $i \geq 1$,

$$(2.2a) \quad p_i = a_i p_{i-1} + p_{i-2},$$

$$(2.2b) \quad q_i = a_i q_{i-1} + q_{i-2},$$

where the recurrence terminates after a finite number of terms in the case that v is rational.

In the remainder of this section we assume that $g_2/N = [0; a_1, \dots, a_k]$, p_i/q_i will denote the i th convergent of g_2/N , and we shall denote

$$m = \min_{i \in \{1, \dots, k\}} (a_i) \quad \text{and} \quad M = \max_{i \in \{1, \dots, k\}} (a_i).$$

It is known (see, for example, [18, Theorem 9]) that, for each $i \in \{1, \dots, k - 1\}$,

$$\left| \frac{g_2}{N} q_i - p_i \right| \leq \frac{1}{q_{i+1}}.$$

From (2.2b) it then follows that

$$(2.3) \quad \left| \frac{g_2}{N} q_i - p_i \right| \leq \frac{1}{a_{i+1} q_i + q_{i-1}} < \frac{1}{a_{i+1} q_i} \leq \frac{1}{m q_i}.$$

Clearly, a small value of m yields, for each q_i , a large upper bound on $|(g_2/N)q_i - p_i|$ in (2.3). It is also known (for example, [18, Theorem 13]) that, for each i ,

$$\left| \frac{g_2}{N} q_i - p_i \right| \geq \frac{1}{q_{i+1} + q_i},$$

and again it follows from (2.2b) that

$$(2.4) \quad \left| \frac{g_2}{N} q_i - p_i \right| \geq \frac{1}{a_{i+1} q_i + q_{i-1} + q_i} \geq \frac{1}{(a_{i+1} + 2) q_i} \geq \frac{1}{(M + 2) q_i}.$$

It follows from (2.4) that for each q_i , that is, for each best approximation, a small value of M yields a large lower bound on $|(g_2/N)q_i - p_i|$. Combining (2.3) and (2.4), we obtain

$$(2.5) \quad \frac{1}{(M + 2) q_i} < \left| \frac{g_2}{N} q_i - p_i \right| < \frac{1}{m q_i}.$$

In effect, these bounds on $|(g_2/N)q_i - p_i| = |(g_2/N) - p_i/q_i|/(1/q_i)$ give estimates of the error of approximation of g_2/N by p_i/q_i , relative to $1/q_i$. In this sense, the first inequality in (2.5) states that a number g_2/N for which M is small is badly approximated by rationals of lower denominator. The following result demonstrates that the denominator q_i of the i th convergent is subject to upper and lower bounds which are monotonic increasing with respect to M and m , respectively. Consequently, for a given value of i , small values of M yield small denominators q_i and small differences between successive denominators.

Lemma 2.1. *With the notation introduced above,*

- (i) $(m + 1)^{(i-1)/2} \leq q_i$ for $i \in \{2, \dots, k\}$, and
- (ii) $q_i \leq (M + 1)^i$ for $i \in \{0, \dots, k\}$.

The proof of (i) with $m = 1$ may be found in [18, Theorem 12] and that of (ii) consists of a straightforward inductive argument, whose details are left to the interested reader.

It follows immediately from Lemma 2.1 that the difference between denominators of successive convergents is bounded by

$$q_{i+1} - q_i \leq (M + 1)^{(i+1)} - (m + 1)^{(i-1)/2},$$

where the expression on the right-hand side of the inequality is monotonic increasing with respect to M . Hence we may expect this difference to be small for small M .

In the two-dimensional case, then, Zaremba’s results lead to the suggestion that vectors \mathbf{g}/N having large values of ρ may be found amongst those possessing the related properties that g_2/N is badly approximated by rationals of lower denominator, and that the best rational approximations to g_2/N have denominators which are not widely separated.

3. BADLY APPROXIMABLE VECTORS AND RANK-1 RULES

In this section a lower bound is established on $\rho(L(\mathbf{g}/N))$ in terms of the closeness of the approximation to the vector $\hat{\mathbf{g}}/N$ given by its best approximating rational vectors of lower denominator, that is, its *best simultaneous approximations*. One interpretation of this result is that good choices of \mathbf{g} and N may be found amongst vectors having the property that $\hat{\mathbf{g}}/N$ is poorly approximated by its best simultaneous approximations, in the sense that, for any given q , the value of $\min_{\mathbf{p} \in \mathbb{Z}^t} \|q\hat{\mathbf{g}}/N - \mathbf{p}\|_\infty$ is large. We then show that vectors $\hat{\mathbf{g}}/N$ having this property may also be characterized as having best simultaneous approximation denominators (*BSADs*) which are not widely separated.

In deriving these results, the following definitions and results from the theory of simultaneous Diophantine approximation will be required. For further details, the interested reader is referred to Cassels [6, Chapter 5] and Lagarias [21].

Definition 3.1 (Lagarias). Let $\mathbf{v} \in \mathbb{R}^t$ and for $q \in \mathbb{N}$ define

$$(3.1) \quad \beta_q(\mathbf{v}) = \min\{\|q\mathbf{v} - \mathbf{p}\| : \mathbf{p} \in \mathbb{Z}^t\},$$

where $\|\cdot\|$ is a given norm on \mathbb{R}^t . The *best simultaneous approximation denominators* (*BSADs*) q_k , where $k \in \mathbb{N}$, for \mathbf{v} with respect to $\|\cdot\|$ are defined by

$$(3.2) \quad q_1 = 1, \quad q_k = \min\{q \in \mathbb{N} : q > q_{k-1}, \beta_q < \beta_{q_{k-1}}\}.$$

The *best simultaneous approximations* (*BSAs*) of \mathbf{v} are the vectors $\mathbf{v}_k = \mathbf{p}_k/q_k \in \mathbb{Q}^t$ for which $\mathbf{p}_k = (p_1^{(k)}, \dots, p_t^{(k)})$ achieves the minimum β_{q_k} in (3.1).

Note that different norms on \mathbb{R}^t may yield different BSADs and BSAs. Also note that if \mathbf{v} is rational, then it has at most a finite number of best approximations $\mathbf{p}_1/q_1, \dots, \mathbf{p}_k/q_k$, say, where $\mathbf{p}_k/q_k = \mathbf{v}$.

Theorem 3.2 (Dirichlet). Let $\mathbf{v} \in \mathbb{R}^t$ and $Q \in \mathbb{R}$ satisfy $Q \geq 1$. Then there exists an integer q and a vector $\mathbf{p} \in \mathbb{Z}^t$ such that $1 \leq q \leq Q$ and

$$\|q\mathbf{v} - \mathbf{p}\|_\infty < Q^{-1/t}.$$

Corollary 3.3. Let \mathbf{p}/q be a BSA of \mathbf{v} . Then $\beta_q(\mathbf{v}) < q^{-1/t}$.

Theorem 3.4. *Let*

$$R_j(\mathbf{x}) = \sum_{i=1}^m \theta_{ji} x_i, \quad S_i(\mathbf{u}) = \sum_{j=1}^n \theta_{ji} u_j,$$

for $1 \leq i \leq m$ and $1 \leq j \leq n$, where $\theta_{ji} \in \mathbb{R}$. Suppose that there is an integer vector $\mathbf{x} \neq \mathbf{0}$ in \mathbb{R}^m and constants C and X such that $0 < C < 1 \leq X$, $\|\mathbf{x}\|_\infty \leq X$ and, for each $j \in \{1, \dots, n\}$,

$$\min_{z \in \mathbb{Z}} |R_j(\mathbf{x}) - z| \leq C.$$

Then there is an integer vector $\mathbf{u} \neq \mathbf{0}$ in \mathbb{R}^n such that for each $i \in \{1, \dots, m\}$

$$\min_{z \in \mathbb{Z}} |S_i(\mathbf{u}) - z| \leq D$$

and $\|\mathbf{u}\|_\infty \leq U$, where

$$\begin{aligned} D &= (l-1)X^{(1-n)/(l-1)}C^{n/(l-1)}, \\ U &= (l-1)X^{m/(l-1)}C^{(1-m)/(l-1)}, \\ l &= m+n. \end{aligned}$$

These results may be used to obtain the following higher-dimensional generalizations of some of the results described in §2.

Theorem 3.5. *Let $\mathbf{p}_1/q_1, \dots, \mathbf{p}_{k-1}/q_{k-1}$ be the successive best approximations of $\hat{\mathbf{g}}/N$, excluding $\hat{\mathbf{g}}/N$ itself. Then*

$$\rho(L(\mathbf{g}/N)) \geq (s-1)^{-(s-1)} \max_{i \in \{1, \dots, k-1\}} (\beta_{q_i}^{s-2} \min(N\beta_{q_i}, q_i)),$$

where $\beta_{q_i} = \|q_i \hat{\mathbf{g}}/N - \mathbf{p}_i\|_\infty$.

Proof. Let $t = s - 1$, as usual, and let

$$B = t^{-t} \max_{i \in \{1, \dots, k-1\}} (\beta_{q_i}^{t-1} \min(N\beta_{q_i}, q_i)).$$

We consider two cases. First, an argument by contradiction shows that, for $\mathbf{h} \in L^\perp - \{\mathbf{0}\}$ such that $\hat{\mathbf{h}} \neq \mathbf{0}$, for each $i \in \{1, \dots, k-1\}$ we cannot have $\|\hat{\mathbf{h}}\|_\infty < q_i \beta_{q_i}^{t-1} t^{-t}$ and $|h_1| < N \beta_{q_i}^t t^{-t}$ simultaneously, and hence that $r(\mathbf{h}) \geq B$, where r is defined in (1.3). Secondly, we show that, if $\mathbf{h} \neq \mathbf{0}$ and $\hat{\mathbf{h}} = \mathbf{0}$, then $r(\mathbf{h}) > B$. The result then follows.

Case (i). Let $\mathbf{h} \in L^\perp$ and $\hat{\mathbf{h}} \neq \mathbf{0}$. Since $\mathbf{h} \in L^\perp$ there exists an integer λ such that

$$\mathbf{g} \cdot \mathbf{h} = 1h_1 + \hat{\mathbf{g}} \cdot \hat{\mathbf{h}} = \lambda N.$$

Assume that there exists an integer $i \in \{1, \dots, k-1\}$ such that both

$$\left| \frac{h_1}{N} \right| = \left| \frac{\hat{\mathbf{g}}}{N} \cdot \hat{\mathbf{h}} - \lambda \right| < \beta_{q_i}^t t^{-t} \quad \text{and} \quad \|\hat{\mathbf{h}}\|_\infty < q_i \beta_{q_i}^{t-1} t^{-t},$$

simultaneously. Now if $q_i \beta_{q_i}^{t-1} t^{-t} \leq 1$, then $\|\hat{\mathbf{h}}\|_\infty = 0$, which contradicts $\hat{\mathbf{h}} \neq \mathbf{0}$. Thus we must have $q_i \beta_{q_i}^{t-1} t^{-t} > 1$. By Corollary 3.3 we have $\beta_{q_i} < q_i^{-1/t}$ and thus $\beta_{q_i}^t < q_i^{-1}$. Consequently, we also have

$$\beta_{q_i}^t t^{-t} < q_i^{-1} t^{-t} \leq 1,$$

since $q_i \geq 1$ and $t \geq 1$, and, by Theorem 3.4, with

$$\begin{aligned} n &= 1, \quad m = t, \quad \theta_i = \hat{g}_i/N, \quad \mathbf{x} = \hat{\mathbf{h}}, \\ C &= \beta_{q_i}^t t^{-t} < 1, \quad 1 \leq X < q_i \beta_{q_i}^{t-1} t^{-t}, \end{aligned}$$

there exists an integer q' such that

$$|q'| \leq U < t(q_i \beta_{q_i}^{t-1} t^{-t})(\beta_{q_i}^t t^{-t})^{(1-t)/t} = q_i$$

and

$$\min_{\mathbf{p} \in \mathbb{Z}^t} \left\| q' \frac{\hat{\mathbf{g}}}{N} - \mathbf{p} \right\|_{\infty} \leq D = t(\beta_{q_i}^t t^{-t})^{1/t} = \beta_{q_i},$$

that is, $\beta_{q'} \leq \beta_{q_i}$. This, however, contradicts the statement that q_i is a BSAD of $\hat{\mathbf{g}}/N$. Consequently, for all $i \in \{1, \dots, k-1\}$, we must have either

$$\|\hat{\mathbf{h}}\|_{\infty} \geq q_i \beta_{q_i}^{t-1} t^{-t} \quad \text{or} \quad |h_1| \geq N \beta_{q_i}^t t^{-t},$$

and, since $r(\mathbf{h}) \geq \max(\|\hat{\mathbf{h}}\|_{\infty}, |h_1|) \geq \min(q_i \beta_{q_i}^{t-1} t^{-t}, N \beta_{q_i}^t t^{-t})$ for $i \in \{1, \dots, k-1\}$, we thus have

$$(3.3) \quad r(\mathbf{h}) \geq t^{-t} \max_{i \in \{1, \dots, k-1\}} (\beta_{q_i}^{t-1} \min(q_i, N \beta_{q_i})) = B.$$

Case (ii). Now let $\|\hat{\mathbf{h}}\| = 0$. Then, since $\mathbf{h} \in L^{\perp} - \{\mathbf{0}\}$, we have $r(\mathbf{h}) = |h_1| = \lambda N$, for some positive integer λ . However, Corollary 3.3 implies that $\beta_{q_i} < 1$, and hence that $B < N$, from (3.3). Thus $r(\mathbf{h}) > B$.

Combining cases (i) and (ii), we observe that $r(\mathbf{h}) \geq B$ for all $\mathbf{h} \in L^{\perp} - \{\mathbf{0}\}$. The result now follows immediately. \square

It is also possible to extract an upper bound on ρ from Theorem 3.4.

Theorem 3.6. *In the notation of Theorem 3.5,*

$$\rho(L(\mathbf{g}/N)) \leq \min_{i \in \{1, \dots, k-1\}} (\max((s-1)^{s-1} q_i, (s-1)^s N q_i^{1/(s-1)} \beta_{q_i})).$$

Proof. As in the proof of Theorem 3.5, we have $\beta_{q_i} < 1$ for $i \in \{1, \dots, k-1\}$. For each value of i , on applying Theorem 3.4 with

$$m = 1, \quad n = t, \quad \theta_j = \hat{g}_j/N, \quad \mathbf{x} = (q_i), \quad C = \beta_{q_i}, \quad X = q_i,$$

we see that there exists an integer vector $\hat{\mathbf{h}} \neq \mathbf{0}$ such that

$$(3.4) \quad \min_{z \in \mathbb{Z}} \left| \frac{\hat{\mathbf{g}}}{N} \cdot \hat{\mathbf{h}} - z \right| \leq D \quad \text{and} \quad \|\hat{\mathbf{h}}\|_{\infty} \leq U,$$

where

$$\begin{aligned} D &= t q_i^{(1-t)/t} \beta_{q_i}^{t/t} = t q_i^{(1-t)/t} \beta_{q_i}, \\ U &= t q_i^{1/t} \beta_{q_i}^{0/t} = t q_i^{1/t} \geq 1. \end{aligned}$$

Hence,

$$(3.5) \quad r(\hat{\mathbf{h}}) \leq \|\hat{\mathbf{h}}\|_{\infty}^t \leq t^t q_i.$$

Now, choose λ to be the integer which achieves the minimum in (3.4) and let $h_1 = \lambda N - \hat{\mathbf{g}} \cdot \hat{\mathbf{h}}$. Then, by (3.4), $|h_1/N| \leq D = t q_i^{(1-t)/t} \beta_{q_i}$, that is,

$$(3.6) \quad |h_1| \leq t q_i^{(1-t)/t} \beta_{q_i} N.$$

TABLE 3.1. Bounds on $\rho(L(\mathbf{g}/N))$. Columns A and B contain respectively the lower and upper bounds given by Theorems 3.5 and 3.6. Columns C and D contain respectively the lower and upper bounds given by Zaremba [47, Propositions 2.1 and 2.2]

s	\mathbf{g}/N	ρ	A	B	C	D
2	$\frac{(10946)}{17711}$	6765	89	6765	5903.7	17711
2	$\frac{(144)}{14489}$	144	89	144	142.0	144.9
3	$\frac{(13581,7739)}{17991}$	392	2.6	5.7709×10^4	–	–
4	$\frac{(14160,9926,5229)}{17580}$	32	40.1	5.8427×10^5	–	–

Computing the product of the bounds on $r(\hat{\mathbf{h}})$ and $|h_1|$ in (3.5) and (3.6), respectively, we then obtain

$$r(\mathbf{h}) = \max(1, |h_1|)r(\hat{\mathbf{h}}) \leq \max(t^t q_i, t^{t+1} N q_i^{1/t} \beta_{q_i}).$$

Since such a vector \mathbf{h} can be constructed for each q_i , it follows that

$$\rho(L(\mathbf{g}/N)) \leq \min_{i \in \{1, \dots, k-1\}} (\max(t^t q_i, t^{t+1} N q_i^{1/t} \beta_{q_i})),$$

and the result follows immediately. □

Example 3.7. The BSAs of $\hat{\mathbf{g}}/N$ may be determined by the simple, if slow, procedure of enumerating the vectors \mathbf{p}/q , for $q \in \{1, \dots, N - 1\}$, which minimize $\|\mathbf{q}\hat{\mathbf{g}}/N - \mathbf{p}\|_\infty$. Table 3.1 summarizes the bounds on $\rho(L(\mathbf{g}/N))$ given by Theorems 3.5 and 3.6, which result from applying this algorithm to a number of choices of $\hat{\mathbf{g}}/N$. In the $s = 2$ case we note that the upper bound on ρ given by Theorem 3.6 is tight, for both choices of $\hat{\mathbf{g}}/N$ considered. In the case of higher dimensions, however, the bounds given by these theorems rapidly become looser since they are based primarily on estimates of $|h_1|$ and $\|\hat{\mathbf{h}}\|_\infty = \max_{i \in \{2, \dots, s\}} |h_i|$ only, rather than taking into account the contribution to $r(\mathbf{h})$ from each component of \mathbf{h} .

Theorems 3.5 and 3.6 provide upper and lower bounds on $\rho(L(\mathbf{g}/N))$ in terms of the BSADs q_1, \dots, q_{k-1} of $\hat{\mathbf{g}}/N$ and the errors of approximation $\beta_{q_1}, \dots, \beta_{q_{k-1}}$ of $\hat{\mathbf{g}}/N$ by its BSAs. One interpretation of the results is that it may be possible to obtain large values of ρ from choices of \mathbf{g} and N which have the property that the values of β_{q_i} and $q_i \beta_{q_i}^{s-2}$ are large, for $1 \leq i \leq k - 1$. Clearly, a vector $\hat{\mathbf{g}}/N$ having the property that $\beta_{q_1}, \dots, \beta_{q_{k-1}}$ are large is not well approximated by rational vectors of lower denominator. It seems reasonable to suggest, therefore, that it may be possible to obtain large values of ρ from vectors \mathbf{g}/N for which $\hat{\mathbf{g}}/N$ is not well approximated by rational vectors of lower denominator. One interpretation (see Theorem 3.10) of the following result suggests that such vectors $\hat{\mathbf{g}}/N$ also possess the property that consecutive BSADs, say q_i and q_{i+1} , are not widely separated, in a particular sense. The proof of Theorem 3.8 is closely based upon the proof by Lagarias [22, proof of Theorem 5.1] of a related result concerning badly approximable irrational vectors.

Theorem 3.8. *Let $N_1 = N/\gcd(g_2, \dots, g_s, N)$, in the notation of Theorem 3.5, and let*

$$(3.7) \quad \begin{aligned} \delta(\hat{\mathbf{g}}/N) &:= \min_{q \in \{1, \dots, N_1-1\}} \beta_q q^{1/t} \\ &= \min_{q \in \{1, \dots, N_1-1\}} \left(\min_{\mathbf{p} \in \mathbb{Z}^t} \left(q^{1/t} \left\| \frac{\hat{\mathbf{g}}}{N} q - \mathbf{p} \right\|_{\infty} \right) \right). \end{aligned}$$

Then $\delta = \delta(\hat{\mathbf{g}}/N) < 1$ and, for $i \in \{1, \dots, k-1\}$,

- (i) $q_i \leq \sum_{j=0}^{i-1} \delta^{-tj} = (\delta^{-ti} - 1)/(\delta^{-t} - 1)$, and
- (ii) $q_{i+1} - q_i < \delta^{-ti}$.

Proof. (i) Clearly we have $\delta > 0$, since $q < N_1$ in (3.7). Also, by Corollary 3.3, $\delta < 1$. For $i \in \{1, \dots, k-1\}$ we must have $q_i < N_1$, since q_i is a BSAD of $\hat{\mathbf{g}}/N$ in its reduced form, and so, from the definition of δ ,

$$(3.8) \quad \delta q_i^{-1/t} \leq q_i^{-1/t} \beta_{q_i} q_i^{1/t} = \beta_{q_i}.$$

Now, by definition we have $q_1 = 1$. Thus for $i \geq 1$ we have $q_{i+1} \geq 2$, or $q_{i+1} - 1 \geq 1$. Applying Theorem 3.2 with $Q = q_{i+1} - 1$ and $\mathbf{v} = \hat{\mathbf{g}}/N$, we see that there exists a positive integer q and an integer vector \mathbf{p} such that $1 \leq q \leq q_{i+1} - 1$ and

$$\beta_q = \|q\hat{\mathbf{g}}/N - \mathbf{p}\|_{\infty} < (q_{i+1} - 1)^{-1/t}.$$

In turn it follows that if $\beta_{q_i} \geq (q_{i+1} - 1)^{-1/t}$, then $\beta_q < \beta_{q_i}$, and thus q must be a BSAD of $\hat{\mathbf{g}}/N$. Furthermore, we must have $q_i < q \leq q_{i+1} - 1$. However, this contradicts the fact that q_i and q_{i+1} are consecutive BSADs, and therefore we must have

$$\beta_{q_i} < (q_{i+1} - 1)^{-1/t}.$$

Hence, by (3.8),

$$\delta q_i^{-1/t} < (q_{i+1} - 1)^{-1/t},$$

and hence

$$(3.9) \quad q_{i+1} < \delta^{-t} q_i + 1.$$

The bound on q_i can now be established by a simple inductive argument. We have $q_1 = 1$ and thus $q_2 < 1 + \delta^{-t}$, by (3.9). Now assume that $q_i \leq \sum_{j=0}^{i-1} \delta^{-tj}$, for some value of i . Then, again by (3.9),

$$q_{i+1} < 1 + \delta^{-t} \sum_{j=0}^{i-1} \delta^{-tj} = \sum_{j=0}^i \delta^{-tj} = \frac{\delta^{-t(i+1)} - 1}{\delta^{-t} - 1},$$

as required.

(ii) Subtracting q_i from both sides of the inequality (3.9) and using the result obtained in (i), we have

$$q_{i+1} - q_i < (\delta^{-t} - 1)q_i + 1 \leq (\delta^{-t} - 1) \frac{\delta^{-ti} - 1}{\delta^{-t} - 1} + 1 = \delta^{-ti}. \quad \square$$

Vectors $\hat{\mathbf{g}}/N$ for which β_q is large, relative to $1/q$, for each $q \in \{1, \dots, N_1 - 1\}$, that is, vectors which are uniformly poorly approximated by rational vectors of lower denominator, yield large values of δ . Since $\delta > 0$ and $t > 0$ it follows that δ^{-t} is a decreasing function of δ , and so large values of δ yield small values of δ^{-t} . Consequently, it follows from Theorem 3.8 that the i th BSAD of a rational vector

which is uniformly poorly approximated by rational vectors of lower denominator is small. In this sense, Theorem 3.8 is a higher-dimensional analogue of Lemma 2.1. It also follows from Theorem 3.8 that consecutive BSADs of vectors which are uniformly poorly approximated are not widely separated. The approximability, by rational vectors of lower denominator, of two rational vectors may be compared in terms of the following definition.

Definition 3.9. Let $N > 0$ and $\mathbf{p}, \mathbf{p}' \in \mathbb{Z}^t$. Let \mathbf{p}, \mathbf{p}' satisfy

$$\gcd(p_1, \dots, p_t, N) = \gcd(p'_1, \dots, p'_t, N) = 1.$$

Then \mathbf{p}/N is *uniformly worse approximable than* \mathbf{p}'/N if for each $q \in \{1, \dots, N-1\}$ we have either

- (i) $\beta_q(\mathbf{p}'/N) < \beta_q(\mathbf{p}/N)$, or
- (ii) $\beta_{q'}(\mathbf{p}'/N) \leq \beta_q(\mathbf{p}/N)$, for some $0 < q' < q$.

Theorem 3.10. Let $\mathbf{p}/N, \mathbf{p}'/N \in \mathbb{Q}^t$ and let

$$\gcd(p_1, \dots, p_t, N) = \gcd(p'_1, \dots, p'_t, N) = 1.$$

Define

$$\begin{aligned} \delta(\mathbf{p}/N) &:= \min_{q \in \{1, \dots, N-1\}} \beta_q(\mathbf{p}/N)q^{1/t}, \\ \delta(\mathbf{p}'/N) &:= \min_{q \in \{1, \dots, N-1\}} \beta_q(\mathbf{p}'/N)q^{1/t}. \end{aligned}$$

If \mathbf{p}/N is *uniformly worse approximable than* \mathbf{p}'/N , then $\delta(\mathbf{p}'/N) < \delta(\mathbf{p}/N)$.

Proof. Let \mathbf{p}/N be uniformly worse approximable than \mathbf{p}'/N . Then for each $q \in \{1, \dots, N-1\}$ we have either $\beta_q(\mathbf{p}'/N) < \beta_q(\mathbf{p}/N)$ or $\beta_{q'}(\mathbf{p}'/N) \leq \beta_q(\mathbf{p}/N)$, for some $0 < q' < q$. If the first condition holds for a given value of q , then clearly $\beta_q(\mathbf{p}'/N)q^{1/t} < \beta_q(\mathbf{p}/N)q^{1/t}$. If, on the other hand, the second condition holds, then we have $\beta_{q'}(\mathbf{p}'/N)q^{1/t} < \beta_{q'}(\mathbf{p}'/N)q^{1/t} \leq \beta_q(\mathbf{p}'/N)q^{1/t}$, for some $q' < q$. Thus, for each $q \in \{1, \dots, N-1\}$ we have, for some $q' \in \{1, \dots, N-1\}$, $\beta_{q'}(\mathbf{p}'/N)q^{1/t} < \beta_q(\mathbf{p}/N)q^{1/t}$, from which it follows that $\delta(\mathbf{p}'/N) < \delta(\mathbf{p}/N)$. \square

From Theorem 3.10 it follows that if $\hat{\mathbf{g}}/N$ is uniformly worse approximable than $\hat{\mathbf{g}}'/N$, then Theorem 3.8 yields a smaller upper bound on the difference between consecutive BSADs of $\hat{\mathbf{g}}/N$ than is the case for $\hat{\mathbf{g}}'/N$.

In the $t = 1$ case, it follows from (2.2b) that $g_2/N = [0; a_1, \dots, a_k]$ is uniformly poorly approximated by rationals of lower denominator if and only if $M = \max_{i \in \{1, \dots, k-1\}}(a_i)$ is small. Thus, Zaremba's results [47, Propositions 2.1 and 2.2] may be interpreted as asserting that a two-dimensional rank-1 simple rule $Q_L(\mathbf{g}/N)$ is good with respect to ρ if and only if $\hat{\mathbf{g}}/N$ is uniformly poorly approximated by rationals of lower denominator.

4. SEQUENCES OF RULES CONSTRUCTED FROM SEQUENCES OF APPROXIMATIONS

If $\mathbf{v} \in \mathbb{R}^t$ is irrational and is badly approximated by rational vectors, then so are all but possibly the first few of its BSAs. This is a consequence of the following theorem, due to Lagarias [22, Lemma 4.1].

Theorem 4.1 (Lagarias). *Let $\mathbf{v} \in \mathbb{R}^t$ and let $\|\cdot\|$ be a norm on \mathbb{R}^t such that*

- (1) *if $\mathbf{p} \in \mathbb{Z}^t - \{\mathbf{0}\}$, then $\|\mathbf{p}\| \geq 1$,*

(2) there exists $\mathbf{p} \in \mathbb{Z}^t$ such that $\|\mathbf{p}\| = 1$.

Let S be a finite set of BSAs (with respect to $\|\cdot\|$) of \mathbf{v} whose largest BSAD is q_k and suppose that $\beta_q < 1/2$ for all elements of S . Then there is an $\epsilon > 0$, depending only on $\mathbf{v}, t, \|\cdot\|$, such that if \mathbf{v}' satisfies $\|\mathbf{v}' - \mathbf{v}\|_\infty < \epsilon$, then the elements of S are also BSAs (with respect to $\|\cdot\|$) of \mathbf{v}' .

Corollary 4.2. Let $\lim_{i \rightarrow \infty} \mathbf{v}_i = \mathbf{v}$ in $(\mathbb{R}^t, \|\cdot\|_\infty)$. Then for each BSA (with respect to $\|\cdot\|_\infty$) of \mathbf{v} , say \mathbf{p}/q , such that $q > 2^t$, there is an $M \in \mathbb{N}$ such that \mathbf{p}/q is a BSA of \mathbf{v}_i for all $i > M$.

Proof. Since $q > 2^t$, so $q^{-1/t} < 1/2$, and hence by Corollary 3.3 we have $\beta_q(\mathbf{v}) < 1/2$. By Theorem 4.1 there is an $\epsilon(\mathbf{v}, t) > 0$ such that $\|\mathbf{v}_i - \mathbf{v}\|_\infty < \epsilon$ implies that \mathbf{p}/q is a BSA of \mathbf{v}_i , from which the result follows. \square

Let $\{\mathbf{p}_i/q_i : 0 < q_i < q_{i+1}\}$ be the sequence of BSAs of \mathbf{v}/N ; then it follows from Corollary 4.2 that each vector \mathbf{p}_i/q_i is also a BSA of later terms in the sequence that have sufficiently large denominators. This suggests that, if $\hat{\mathbf{g}}/N$ is a BSA of a badly approximable vector, then it is itself likely to be badly approximated by rational vectors of lower denominator, and so are all but possibly the first few of its BSAs. This is a slightly weakened higher-dimensional analogue of the properties that, in the case where $t = 1$ (that is, in the one-dimensional approximation problem),

- (1) the best approximations to a rational number $v = [a_0; a_1, \dots, a_k]$, where $a_k > 1$, are the principal convergents $p_0/q_0, p_1/q_1, \dots, p_k/q_k$, except for possibly the first convergent p_0/q_0 ,
- (2) the best approximations to each convergent p_i/q_i are (with the possible exception of p_0/q_0) the preceding convergents, and
- (3) if v is badly approximated by rationals of lower denominator, and in particular by its convergents, then the relationship between the continued fraction for v and the continued fractions for its convergents clearly implies that each of the principal convergents of v is itself poorly approximated.

Theorem 4.1 does not restrict \mathbf{v} to be a rational vector, and thus the observations that derive from it may also be applied to irrational vectors, with the obvious modification that such vectors have infinitely many rational BSAs. In the $t = 1$ case this observation, together with Zaremba's results, shows how an infinite sequence of good rank-1 lattice rules may be constructed from the sequence of best approximations to the irrational limit of a suitably chosen convergent continued fraction. The well-known Fibonacci rules described by (1.7a) and (1.7b) form just such sequences. The observations of this section raise the question of whether sequences of good rules can be constructed in higher dimensions from the BSAs of irrational vectors which are badly approximated by rational vectors.

Informally, an irrational vector \mathbf{v} is badly approximated by rational vectors if the error of approximation by any rational vector \mathbf{p}/q is large relative to $1/q$, except for at most a finite number (depending on \mathbf{v}) of such approximations. More precisely, it is known that for each $t > 0$ there are vectors $\mathbf{v} \in \mathbb{R}^t$ with the property that there exists a $c > 0$ such that $\lim_{q \rightarrow \infty} \inf\{q^{1/t} \|\mathbf{q}\mathbf{v} - \mathbf{p}\|_\infty : \mathbf{p} \in \mathbb{Z}^t\} > c$. Such vectors are said to be *badly approximable*, and we may compare the approximability, in this sense, of two such vectors, \mathbf{v}_1 and \mathbf{v}_2 say, by comparing $\bar{\delta}(\mathbf{v}_1)$ and $\bar{\delta}(\mathbf{v}_2)$, where

$$\bar{\delta}(\mathbf{v}) = \liminf_{q \rightarrow \infty} \beta_q q^{1/t} > 0.$$

For $t = 1$ the chain of largest values of $\bar{\delta}(v)$ in \mathbb{R} and the continued fractions for the corresponding values of v are well known (see, for example, [8]). There is a substantial literature devoted to the open problem of determining, for given $t > 1$, the largest such constant $\bar{\delta}$ (see, for example, [45]). Theorems 3.5, 3.6 and 3.10 suggest, however, that our interest should lie not in the asymptotic badness of the approximability of \mathbf{v}_1 and \mathbf{v}_2 , but rather in the comparative badness of their initial BSAs. For this reason, not every badly approximable vector yields good choices of $\hat{\mathbf{g}}$ and N , at least for small values of N . Thus, we choose $\delta(\mathbf{v})$ as defined in (3.7), rather than $\bar{\delta}(\mathbf{v})$, as a guide to choosing \mathbf{v} , reflecting an emphasis on uniformly bad approximation rather than asymptotic bad approximability.

In the one-dimensional case, numbers that are badly approximable are characterized as having continued fraction expansions with bounded elements. Furthermore, the continued fraction algorithm itself yields a convenient method for computing best approximations to numbers which are known to be poorly approximated, without knowing these numbers a priori. In higher dimensions, it is known that certain types of vectors are poorly approximated by rationals—for example, vectors whose components constitute an integral basis for a real algebraic field (see, for example, [36, Chapter 2, Theorem 4a]). However, the author is not aware of any characterization of badly approximable vectors of arbitrary dimension which yields a convenient method for computing their BSAs.

In a related result, Hua and Wang [15, Lemmas 7.5 and 7.6] assert that good rational approximations to certain integral bases for real algebraic fields may be used to construct rules with a particular lower bound on ρ . The results of Hua and Wang deal with ‘good’ approximations to integral bases, not with best approximations. This raises the more general questions of whether sequences of good rules may be constructed from good approximations to given badly approximable vectors, and of how we may compute a priori good rational approximations to vectors which are likely to be badly approximable. To answer the first of these questions, we first formalize the notion of ‘good approximation’ and then prove a ‘transference’ property for good approximations that is analogous to that expressed by Corollary 4.2 for BSAs. We defer consideration of the second question until §5.

Definition 4.3. Let $\mathbf{v} \in \mathbb{R}^t$, $\mathbf{p} \in \mathbb{Z}^t$, $q \in \mathbb{N}$ and let ν be a positive real number. Then \mathbf{p}/q is a ν -good approximation to \mathbf{v} if

$$\|\mathbf{v} - \mathbf{p}/q\|_\infty < \nu q^{-(1+1/t)}.$$

We may use arguments similar to those used to establish Theorem 4.1 and Corollary 4.2 to obtain the following, somewhat weaker, results for ν -good approximations.

Theorem 4.4. Let $\mathbf{v} \in (\mathbb{R}^t, \|\cdot\|_\infty)$ and let \mathbf{p}/q be a ν -good approximation to \mathbf{v} . Then there exists an $\epsilon > 0$, depending only on \mathbf{v}, t, ν, q , such that if $\|\mathbf{v} - \mathbf{v}'\|_\infty < \epsilon$, then \mathbf{p}/q is a ν -good approximation to \mathbf{v}' .

Proof. Let $d = \|q\mathbf{v} - \mathbf{p}\|_\infty$; then $d < \nu q^{-1/t}$. Let $\mathbf{w} = \mathbf{v}' - \mathbf{v}$; then $\|q(\mathbf{v} + \mathbf{w}) - \mathbf{p}\|_\infty \leq \|q\mathbf{v} - \mathbf{p}\|_\infty + \|q\mathbf{w}\|_\infty < \nu q^{-1/t}$, when $\|\mathbf{w}\|_\infty < (\nu q^{-1/t} - d)/q$. Choosing $\epsilon = (\nu q^{-1/t} - d)/q$, we observe that, if $\|\mathbf{v} - \mathbf{v}'\|_\infty < \epsilon$, then \mathbf{p}/q is a ν -good approximation to \mathbf{v}' . \square

Corollary 4.5. *Let $\lim_{i \rightarrow \infty} \mathbf{v}_i = \mathbf{v}$ in $(\mathbb{R}^t, \|\cdot\|_\infty)$. For each ν -good approximation, say \mathbf{p}/q , to \mathbf{v} there exists an $M \in \mathbb{N}$ such that \mathbf{p}/q is a ν -good approximation of \mathbf{v}_i for all $i > M$.*

If $\{\mathbf{p}_1/q_1, \mathbf{p}_2/q_2, \dots\}$ is a sequence of ν -good approximations to a vector \mathbf{v} with $q_i > 0$ and $q_i < q_{i+1}$, then it follows from Corollary 4.5 that each vector \mathbf{p}_i/q_i is also a ν -good approximation to later terms in the sequence that have sufficiently large denominators. Clearly, it also follows that if \mathbf{v} is poorly approximated by rational vectors, then so are its ν -good approximations, for sufficiently large denominators and sufficiently small ν . Since, as we have already noted, it is known that a vector \mathbf{v} whose elements form an integral basis for a real algebraic field is badly approximable, this observation provides some justification for the suggestion that sequences of ‘good’ approximations to such vectors might be used to construct sequences of good rank-1 lattice rules. As previously noted, however, the results of §3 suggest that the choice of \mathbf{v} must be made with some care to ensure that it is uniformly badly approximable, in the sense that $\delta(\mathbf{v}) = \inf\{\beta_q q^{1/t} : q > 0\} < 1$ is large.

Lemmas 7.5 and 7.6 of Hua and Wang [15] state lower bounds for ρ in the case of certain 1-good approximations to integral bases for two particular fields. The numerical results reported in the tables of [15] and our own preliminary investigations (see Tables 6.1, 6.2 and Tables A.1–A.6 of the appendix on the microfiche card attached to this issue) reveal that, in practice, the quality of rules constructed from a sequence of approximations to any single such vector may vary considerably with respect to the parameter z_s defined in (1.5), which provides a measure of the quality of ρ with respect to the size of N . Thus, we may hope to obtain better rules on average by compiling a list of the best rules obtained by considering approximations to many badly approximable vectors, rather than by considering the approximations to only a few such vectors.

The results of this section indicate that we may find best and ν -good approximations to badly approximable irrational vectors amongst those of rational vectors sufficiently close to them—that is, the properties of badly approximable irrational vectors in which we are interested are, in a sense, inherited by their best and, to a lesser extent, their ν -good rational approximations. Similarly, the limit of a convergent sequence of rational vectors, the terms of which are best approximations or ν -good approximations to later terms and which share the properties of being poorly approximated by rational vectors of lower denominator and having consecutive BSADs which are not widely separated, will itself inherit these properties. In this sense, Theorem 3.5 suggests the possibility of a computational scheme for searching for good choices of $\hat{\mathbf{g}}/N$ amongst good approximations to a number of uniformly poorly approximable (rational or irrational) vectors. Such a scheme may be constructed from:

- (i) a characterization of such vectors in terms of a computationally convenient criterion, and
- (ii) an efficient method for computing good approximations to the vectors chosen, or constructed, according to this criterion.

Theorem 3.8 answers the first requirement in terms of the spacing between successive BSADs. As we have already noted, it suggests that we should consider vectors whose successive BSADs are not widely separated. In the following section we present a partial answer to the second requirement.

5. ADAPTATION OF THE SZEKERES CONTINUED FRACTION ALGORITHM

Convenient methods for computing sequences of good rational approximations to *known* $\mathbf{v} \in \mathbb{R}^t$ are afforded by the methods of Szekeres [44] and Brentjes [4]. Various descriptions of the Szekeres algorithm are available ([4], [7], [44]). The Brentjes algorithm is described in depth for the special case $t = 2$ in [5]. Lagarias [21] observes that the Szekeres algorithm performs, in general, very well, although it does not find all uniform-norm best approximations for arbitrary \mathbf{v} —both he and Brentjes [4] exhibit counterexamples. Cusick [7] showed that the Szekeres algorithm finds all best approximations to zero by the linear form $x_0 + x_1(\phi^2 - 1) + x_2(\phi - 1)$, where $\phi = 2 \cos(2\pi/7)$ generates the real cyclotomic field \mathfrak{R}^3 of degree three, and $\{1, \phi^2 - 1, \phi - 1\}$ is an integral basis of \mathfrak{R}^3 . Brentjes [5] proved that his algorithm finds all Euclidean-norm best approximations in two dimensions, using a modified definition of the notion of ‘best approximation’. In this work, we are concerned only with Szekeres’ algorithm and in the remainder of this section we largely follow his notation.

Given $\mathbf{v} \in \mathbb{R}^t$ and an initial $(t + 1) \times (t + 1)$ matrix \mathfrak{A}_0 , the Szekeres algorithm determines a sequence $\{\epsilon_k\}$ of binary-valued *switching flags* (there is a switch from the current approximation direction to a new direction if and only if $\epsilon_{k+1} = 1$), a sequence $\{s_m\}$ of *switching values*, the elements of which are the values of k at which $\epsilon_k = 1$, and a sequence of integer *elements* $\{b_m\}$, which correspond to the elements of a one-dimensional simple continued fraction, given by

$$(5.1) \quad b_1 = s_1, \quad b_m = s_m - s_{m-1}, \quad m > 1.$$

The elements b_1, b_2, \dots represent the numbers of approximation steps between successive switching points. Given an initial matrix \mathfrak{A}_0 , the algorithm also determines a sequence of $(t + 1) \times (t + 1)$ *approximation matrices* \mathfrak{A}_k , whose rows and columns are indexed from 0 to t . We denote by $A^{(i)}(k, j)$ the entry in row i and column j of \mathfrak{A}_k . For each approximation matrix a column (labelled by the index μ) is selected. The entries in that column of the succeeding approximation matrix form the next *approximation vector*, represented by the pair (B_k, \mathbf{A}_k) say, where $B_k = A^{(0)}(k, \mu(k - 1))$ and $\mathbf{A}_k = (A^{(1)}(k, \mu(k - 1)), \dots, A^{(t)}(k, \mu(k - 1)))$. The vector \mathbf{A}_k/B_k is the approximation to \mathbf{v} . The vectors (Q_m, \mathbf{P}_m) , where

$$(5.2) \quad Q_m = A^{(0)}(s_m, 0) \text{ and } \mathbf{P}_m = (A^{(1)}(s_m, 0), \dots, A^{(t)}(s_m, 0)),$$

are called *principal approximation vectors*. The last principal approximation vector found at the k th stage of the algorithm is stored in the initial column of \mathfrak{A}_k (labelled with index 0). The algorithm is designed so that the principal approximations should contain the best approximations, in a particular sense, that it finds—the values of ϵ_k are chosen precisely to ensure that the successive best approximations found by the algorithm are ‘switched’ into the initial column at the appropriate points during processing. The symbol $[b_1, b_2, \dots, b_m]$ represents the principal approximation vector (Q_m, \mathbf{P}_m) and is called the t -fraction for (Q_m, \mathbf{P}_m) . The symbol $[b_1, b_2, \dots]$ represents the corresponding sequence of principal approximation vectors and is called the t -fraction for $\mathbf{v} = \lim_{m \rightarrow \infty} \mathbf{P}_m/Q_m$. The reader is referred to [44] for further details.

Successive approximation matrices are computed according to the equations

$$(5.3) \quad A^{(i)}(k+1, 0) = (1 - \epsilon_{k+1})A^{(i)}(k, 0) + \epsilon_{k+1}A^{(i)}(k, \mu(k)),$$

$$(5.4) \quad A^{(i)}(k+1, \mu(k)) = A^{(i)}(k, 0) + A^{(i)}(k, \mu(k)),$$

$$(5.5) \quad A^{(i)}(k+1, j) = A^{(i)}(k, j), \quad 1 \leq j \leq t, \quad j \neq \mu(k),$$

for $i = 0, 1, \dots, t$. The k th approximation vector is chosen from the columns of \mathfrak{A}_k according to the selection rule:

$$(5.6) \quad \mu(k) = \max\{j : 1 \leq j \leq t, \|\mathbf{E}_j\|_\infty \geq \|\mathbf{E}_{j'}\|_\infty \text{ for all } j' = 1, 2, \dots, t\},$$

where $\mathbf{E}_j = \mathbf{M}_j/A^{(0)}(k, j) - \mathbf{A}_k/B_k$ and $\mathbf{M}_j = (A^{(1)}(k, j), \dots, A^{(t)}(k, j))$.

It is evident from this description that the calculation of \mathfrak{A}_k depends on the value of ϵ_k having been determined. In Szekeres' formulation of the algorithm, this value is determined on the basis of knowledge of both \mathbf{v} and \mathfrak{A}_{k-1} . In our case, however, \mathbf{v} is presumed unknown. Nevertheless, if an infinite sequence of elements $\{b_m\}$ and an initial matrix \mathfrak{A}_0 are given, then sequences $\{s_m\}$ and $\{\epsilon_k\}$ are determined by (5.1) and a sequence of vectors $\{\mathbf{P}_m/Q_m\}$ is determined by (5.2)–(5.6) which converges, by the argument of Szekeres [44, Theorems 4], [8], to some $\mathbf{v} \in \mathbb{R}^t$. If \mathfrak{A}_0 is an integer matrix, then \mathbf{A}_k/B_k is a rational vector, for each $k \in \mathbb{N}$.

It remains to identify a set of t -fractions which are likely to converge to badly approximable vectors. In practice, the set of principal approximations of a t -fraction which converges to \mathbf{v} , say, contains those uniform-norm best approximations to \mathbf{v} found by the Szekeres algorithm (see the examples in [21] and [44]). It would appear, therefore, that the simplest criterion to apply in identifying a suitable set of t -fractions is that the denominators of successive principal approximations should increase slowly. The relationship between successive principal approximations defined by (5.1)–(5.6) leads to the following result.

Theorem 5.1. *Let the t -fraction $[b_1, b_2, \dots]$ have initial matrix \mathfrak{A}_0 , where*

$$A^{(i)}(0, j) = \begin{cases} 1 & \text{if } i \leq j, \\ 0 & \text{if } i > j, \end{cases}$$

and let $b_m \leq M$ for all $m \in \mathbb{N}$. Then for all $m \in \mathbb{N}$, the denominator Q_m of the m th principal approximation vector satisfies

$$(5.7) \quad Q_m \leq (M + 1)^m.$$

Proof. We consider the derivation of (Q_m, \mathbf{P}_m) from $(Q_{m-1}, \mathbf{P}_{m-1})$ via (5.1)–(5.6). Define $s_0 = 0$; then from (5.1) we have $s_m = s_{m-1} + b_m$ for $m \geq 1$. Also, for $k = 1, 2, \dots, b_m - 1$, we have $\epsilon_{s_{m-1}+k} = 0$ and equations (5.3)–(5.5) yield

$$\begin{aligned} A^{(i)}(s_{m-1} + k, 0) &= A^{(i)}(s_{m-1} + k - 1, 0), \\ A^{(i)}(s_{m-1} + k, \mu(s_{m-1} + k - 1)) &= A^{(i)}(s_{m-1} + k - 1, 0) \\ &\quad + A^{(i)}(s_{m-1} + k - 1, \mu(s_{m-1} + k - 1)), \\ A^{(i)}(s_{m-1} + k, j) &= A^{(i)}(s_{m-1} + k - 1, j), \quad j \neq \mu(s_{m-1} + k - 1), \end{aligned}$$

for $i = 0, 1, \dots, t$. Thus, for $k = 1, \dots, b_m - 1$,

$$(5.8) \quad \mathfrak{A}_{s_{m-1}+k} = \mathfrak{A}_{s_{m-1}+k-1} \mathbf{E}_{m,k},$$

where $\mathbf{E}_{m,k}$ is the elementary matrix which, when postmultiplying $\mathfrak{A}_{s_{m-1}+k-1}$, adds the column 0 to the column $\mu(s_{m-1} + k - 1)$. For $k = b_m$, we recall that $s_{m-1} + k = s_m$ and $\epsilon_{s_m} = 1$, whence we obtain, from (5.3)–(5.5),

$$\begin{aligned} A^{(i)}(s_m, 0) &= A^{(i)}(s_m - 1, \mu(s_m - 1)), \\ A^{(i)}(s_m, \mu(s_m - 1)) &= A^{(i)}(s_m - 1, 0) + A^{(i)}(s_m - 1, \mu(s_m - 1)), \\ A^{(i)}(s_m, j) &= A^{(i)}(s_m - 1, j), \quad 1 \leq j \leq t, \quad j \neq \mu(s_m - 1), \end{aligned}$$

for $i = 0, 1, \dots, t$. It follows that

$$(5.9) \quad \mathfrak{A}_{s_m} = \mathfrak{A}_{s_{m-1}} \mathbf{E}_{m,b_m} \mathbf{F}_m,$$

where \mathbf{E}_{m,b_m} is defined in a manner analogous to $\mathbf{E}_{m,k}$ for $k < b_m$, and

$$\mathbf{F}_m = \begin{pmatrix} -1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 1 & & \mathbf{I}_t & \\ 0 & & & \\ \vdots & & & \\ 0 & & & \end{pmatrix},$$

where the unit elements in the initial column occur in rows 0 and $\mu(s_m - 1)$, and \mathbf{I}_t is the $t \times t$ identity matrix. It now follows from (5.8) and (5.9) that

$$(5.10) \quad \mathfrak{A}_{s_m} = \mathfrak{A}_{s_{m-1}} \mathbf{C}_m \mathbf{F}_m,$$

where $\mathbf{C}_m = \prod_{k=1}^{b_m} \mathbf{E}_{m,k}$ has the form

$$\mathbf{C}_m = \begin{pmatrix} 1 & c_{m,1} & c_{m,2} & \cdots & c_{m,t} \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & & \cdots & & 1 \end{pmatrix},$$

with $c_{m,j} \geq 0$ and $\sum_{j=1}^t c_{m,j} = b_m$. We thus obtain

$$A^{(0)}(s_m, 0) = A^{(0)}(s_{m-1}, \mu(s_m - 1)) + (c_{m,\mu(s_m-1)} - 1)A^{(0)}(s_{m-1}, 0),$$

and, for $1 \leq j \leq t$,

$$A^{(0)}(s_m, j) = c_{m,j}A^{(0)}(s_{m-1}, 0) + A^{(0)}(s_{m-1}, j).$$

An inductive argument now yields the result—in particular, we establish that

$$(5.11) \quad A^{(0)}(s_m, j) \leq (M + 1)^m$$

for $0 \leq j \leq t$. For $m = 1$, we observe that

$$A^{(0)}(s_1, j) = \begin{cases} c_{1,\mu(s_1-1)} & \text{for } j = 0, \\ 1 + c_{1,j} & \text{for } 1 \leq j \leq t, \end{cases}$$

and, since $c_{1,j} \leq M$, (5.11) holds. In general, if (5.11) holds for $m = n$, say, then for $1 \leq j \leq t$,

$$\begin{aligned} A^{(0)}(s_{n+1}, j) &= c_{n+1,j}A^{(0)}(s_n, 0) + A^{(0)}(s_n, j) \\ &\leq M(M + 1)^n + (M + 1)^n = (M + 1)^{n+1}, \end{aligned}$$

and, for $j = 0$,

$$\begin{aligned} A^{(0)}(s_{n+1}, 0) &= A^{(0)}(s_n, \mu(s_{n+1} - 1)) + (c_{n+1,\mu(s_{n+1}-1)} - 1)A^{(0)}(s_n, 0) \\ &\leq (M + 1)^n + M(M + 1)^n = (M + 1)^{n+1}. \end{aligned}$$

The inequality (5.7) now follows immediately, which completes the proof. □

In light of the remarks in §§3 and 4, Theorem 5.1 provides some justification for searching for generators of good rank-1 lattice rules amongst the approximation vectors generated by finite t -fractions whose elements satisfy a small upper bound. In the following section we present the results of a number of such search strategies. In these searches the Euclidean norm, rather than the uniform norm, was used in the selection rule μ as defined by (5.6), since slightly better results were obtained in preliminary studies using this norm.

6. NUMERICAL RESULTS

As we have noted in §1, in the case of two-dimensional lattice rules it is known [47] that the Fibonacci rules specified by (1.7) are the best possible rank-1 rules, in the sense that, for $k \geq 5$, the values of z_2 exceed $10/29$, whereas the maximum value of z_2 attained by any other two-dimensional rank-1 lattice rule is $10/29$. Further investigation of the two-dimensional case reveals that, at least for $N < 10000$, every rank-1 simple lattice rule $Q_{L(\mathbf{g}/N)}$ such that, if $\text{order}(Q_{L'}) < N$, then $\rho(L') < \rho(L)$, also has the property that $M \leq 2$, where M is the maximum element in the continued fraction for g_2/N . As noted in §1, a number of authors also use P_α as a figure of merit, and for these reasons we introduce the following terms.

Definition 6.1. An s -dimensional lattice rule Q_L of order N will be called *bestP₂* with respect to a set S of lattice rules if, for every $Q_{L'} \in S$:

- (1) if $\text{order}(Q_{L'}) < N$, then $P_2(Q_{L'}) > P_2(Q_L)$, and
- (2) if $\text{order}(Q_{L'}) = N$, then $P_2(Q_{L'}) \geq P_2(Q_L)$.

Definition 6.2. An s -dimensional lattice rule Q_L of order N will be called *bestρ* with respect to a set S of lattice rules if, when $Q_{L'} \in S$:

- (1) if $\text{order}(Q_{L'}) < N$, then $\rho(L') < \rho(L)$, and
- (2) if $\text{order}(Q_{L'}) = N$, then $\rho(L') \leq \rho(L)$.

There are a number of important differences between the two-dimensional case and that of higher dimensions. First, for $s > 2$, the worst approximable vector in \mathbb{R}^{s-1} is not known, and secondly, there is no complete analogue of the one-dimensional continued fraction algorithm (cf. [21]). Indeed, it seems probable that there is not, in general, a single vector \mathbf{v} amongst whose good approximations are to be found rational vectors $\hat{\mathbf{g}}/N$ producing lattice generators \mathbf{g}/N which are uniformly best possible, in the sense of having z_s -values exceeding those of other rank-1 simple lattice rules.

For brevity, we shall say that, if $\hat{\mathbf{g}}/N$ is a Szekeres approximation fraction for $\mathbf{v} \in \mathbb{R}^{s-1}$, then the s -dimensional lattice rule Q_L is *induced by the $(s-1)$ -fraction \mathbf{v}* .

Let V_1 and V_2 denote the sets of three-dimensional rank-1 simple rules induced by Szekeres approximations of $\mathbf{v}_1 = [1, 1, \dots]$ and $\mathbf{v}_2 = (4\phi^2 - 1, 2\phi - 1)$, respectively, where $\phi = \cos(2\pi/7)$ is the generator of the real cyclotomic field \mathfrak{R}^3 of degree three used to obtain the last two entries in Table 2 of Hua and Wang [15]. Tables 6.1 and 6.2 list the best P_2 rules (with respect to V_1 and V_2 , respectively) of order not exceeding 1000000. It is conjectured by Szekeres [45] that \mathfrak{R}^3 contains the worst approximable pairs of irrationals. Nevertheless, it is apparent that neither sequence of rules is uniformly superior to the other with respect to z_3 , and in both cases the values of z_3 obtained vary considerably with N .

The three-dimensional rules listed in Table 6.1 for \mathbf{v}_1 do, however, compare favorably with those obtained by Hua and Wang [15, Table 2] from their approximations to \mathbf{v}_2 , although they obtain better results than some of those obtained by applying the Szekeres algorithm directly to \mathbf{v}_2 . In particular, they obtain rules for which $\rho = 1411$, $P_2 = 3.33 \times 10^{-6}$ and $z_3 = 0.119$ at $N = 140052$, and $\rho = 2696$, $P_2 = 1.23 \times 10^{-6}$ and $z_3 = 0.108$ at $N = 314694$, whereas for \mathbf{v}_1 we obtain $\rho = 1974$, $P_2 = 2.09 \times 10^{-6}$ and $z_3 = 0.180$ at $N = 128801$; $\rho = 3710$, $P_2 = 1.04 \times 10^{-6}$ and $z_3 = 0.262$ at $N = 170625$; and $\rho = 3428$, $P_2 = 5.30 \times 10^{-7}$ and $z_3 = 0.144$ at $N = 299426$. For \mathbf{v}_2 we obtain $\rho = 1086$, $P_2 = 5.89 \times 10^{-6}$ and $z_3 = 0.094$ at $N = 137068$; $\rho = 1086$, $P_2 = 4.62 \times 10^{-6}$ and $z_3 = 0.077$ at $N = 170921$; $\rho = 2628$, $P_2 = 1.35 \times 10^{-6}$ and $z_3 = 1.32$ at $N = 246988$; and $\rho = 2438$, $P_2 = 1.11 \times 10^{-6}$ and $z_3 = 0.082$ at $N = 384056$. Comparison of the rules in Tables 6.1 and 6.2 with the 3-*D* Fibonacci and *A, N*-type rules in Worley [46] reveals that, for large orders, those in Tables 6.1 and 6.2 are markedly better with respect to both ρ and P_2 .

Similar comparisons may be made between the results obtained via the methods of Hua and Wang [15] and those obtained by constructing lattice generators from approximations to the Szekeres $(s-1)$ -fraction $[1, 1, \dots]$ for $s > 3$. Tables A.1–A.6 of the Appendix list the best P_2 rules obtained in this way for dimensions 4 to 9. For $3 \leq s \leq 9$ the rules obtained by the method of Hua and Wang and marked in their Tables 3–8 by an asterisk (*) are superior, with respect to P_2 , to those induced by the $(s-1)$ -fraction $[1, 1, \dots, 1]$, except in the cases $s = 3$ and $s = 5$. Nevertheless, the fluctuation in the values of z_s for the latter rules suggests that better results might be obtained by compiling a list of the best rules induced by approximations to some larger set of vectors.

The method of Hua and Wang does not lend itself easily to such a scheme, since it is not obvious how to characterize a suitable set of vectors. However, the discussion in §5 suggests that a suitable set may consist of vectors with $(s-1)$ -fractions having elements subject to a small upper bound. Let S denote the set of three-dimensional rules of order not exceeding 1000 induced by 2-fractions $[b_1, b_2, \dots, b_{20}]$ satisfying $b_i \leq 2$. Table 6.3 lists those rules which are best ρ with respect to S —note that, following the convention of earlier authors, only rules which are not geometrically equivalent, that is, are not obtainable from other rules in the list by a symmetry of the cube U^s , are listed. Comparison with Table 9 of Maisonneuve [28] reveals that those which appear with an asterisk in Table 6.3 are also best ρ with respect to the set of all rank-1 simple three-dimensional rules. Indeed, an exhaustive search of all (including nonsimple) rank-1, three-dimensional lattice rules indicates that the rules with $N = 66, 650, 737$ and 882 are best ρ with respect to this larger set as well.

At least in dimension three, then, $(s-1)$ -fractions with elements subject to a small upper bound M , say, induce some very good rules. Even with $M = 2$,

TABLE 6.1. Best P_2 rules derived from approximations to $\mathbf{v}_1 = [1, 1, \dots] \in \mathbb{R}^s$: $s = 3$

N	ρ	z_s	P_2	P_4	\mathbf{g}
9	2	4.88e-01	6.97e+00	8.80e-01	1 7 4
12	2	4.14e-01	5.06e+00	6.02e-01	1 9 5
16	2	3.47e-01	3.60e+00	3.54e-01	1 12 7
21	2	2.90e-01	2.50e+00	2.00e-01	1 16 9
28	3	3.57e-01	1.62e+00	6.54e-02	1 21 12
37	4	3.90e-01	1.12e+00	3.20e-02	1 28 16
49	4	3.18e-01	7.24e-01	1.44e-02	1 37 21
65	4	2.57e-01	5.26e-01	1.08e-02	1 49 28
86	7	3.63e-01	3.16e-01	2.30e-03	1 65 37
114	7	2.91e-01	2.19e-01	1.61e-03	1 86 49
151	12	3.99e-01	1.28e-01	3.16e-04	1 114 65
200	14	3.71e-01	8.85e-02	1.82e-04	1 151 86
265	14	2.95e-01	5.84e-02	9.48e-05	1 200 114
351	14	2.34e-01	4.05e-02	6.95e-05	1 265 151
465	14	1.85e-01	2.97e-02	6.13e-05	1 351 200
616	14	1.46e-01	2.30e-02	5.85e-05	1 465 265
816	14	1.15e-01	1.97e-02	5.77e-05	1 616 351
1081	25	1.62e-01	9.36e-03	8.52e-06	1 816 465
1432	25	1.27e-01	8.26e-03	8.46e-06	1 1081 616
1897	42	1.67e-01	3.38e-03	9.86e-07	1 1432 816
2513	50	1.56e-01	2.41e-03	5.38e-07	1 1897 1081
3329	70	1.71e-01	1.36e-03	1.51e-07	1 2513 1432
4410	98	1.86e-01	7.83e-04	4.35e-08	1 3329 1897
5842	125	1.86e-01	4.96e-04	1.69e-08	1 4410 2513
7739	168	1.94e-01	2.84e-04	4.95e-09	1 5842 3329
10252	224	2.02e-01	1.85e-04	1.83e-09	1 7739 4410
13581	294	2.06e-01	1.03e-04	5.59e-10	1 10252 5842
17991	392	2.13e-01	7.38e-05	2.45e-10	1 13581 7739
23833	518	2.19e-01	3.58e-05	5.95e-11	1 17991 10252
31572	686	2.25e-01	2.44e-05	2.48e-11	1 23833 13581
41824	910	2.32e-01	1.25e-05	6.36e-12	1 31572 17991
55405	1204	2.37e-01	7.71e-06	2.19e-12	1 41824 23833
73396	1596	2.44e-01	4.43e-06	6.93e-13	1 55405 31572
97229	2114	2.50e-01	2.92e-06	2.96e-13	1 73396 41824
128801	1974	1.80e-01	2.09e-06	1.97e-13	1 97229 55405
170625	3710	2.62e-01	1.04e-06	4.42e-14	1 128801 73396
299426	3428	1.44e-01	5.30e-07	5.33e-15	1 226030 128801
525456	6014	1.51e-01	2.35e-07	5.33e-15	1 396655 226030
922111	3428	5.11e-02	2.32e-07	2.00e-14	1 696081 396655

TABLE 6.2. Best P_2 rules in \mathbb{R}^3 derived from approximations to $\mathbf{v}_2 = (4\phi^2 - 1, 2\phi - 1)$ generated by the Szekeres algorithm with $\phi = \cos \frac{2\pi}{7}$

N	ρ	z_s	P_2	P_4	\mathbf{g}
9	2	4.88e-01,	6.97e+00	8.80e-01	1 5 2
11	2	4.36e-01,	5.48e+00	6.26e-01	1 6 3
16	2	3.47e-01,	3.60e+00	3.54e-01	1 9 4
20	2	3.00e-01,	2.90e+00	3.00e-01	1 11 5
25	2	2.58e-01,	2.03e+00	1.65e-01	1 14 6
36	4	3.98e-01,	1.20e+00	3.84e-02	1 20 9
45	4	3.38e-01,	9.85e-01	3.15e-02	1 25 11
65	4	2.57e-01,	5.95e-01	1.46e-02	1 36 16
81	4	2.17e-01,	4.29e-01	9.79e-03	1 45 20
101	4	1.83e-01,	3.47e-01	8.90e-03	1 56 25
146	8	2.73e-01,	1.72e-01	1.05e-03	1 81 36
182	8	2.29e-01,	1.33e-01	8.90e-04	1 101 45
227	9	2.15e-01,	9.34e-02	4.55e-04	1 126 56
328	16	2.83e-01,	4.84e-02	8.00e-05	1 182 81
409	18	2.65e-01,	3.76e-02	5.64e-05	1 227 101
591	18	1.94e-01,	2.24e-02	2.81e-05	1 328 146
737	18	1.61e-01,	1.72e-02	2.27e-05	1 409 182
919	18	1.34e-01,	1.40e-02	2.10e-05	1 510 227
1328	18	9.75e-02,	1.09e-02	2.01e-05	1 737 328
1656	18	8.06e-02,	9.62e-03	1.99e-05	1 919 409
2065	18	6.65e-02,	8.83e-03	1.98e-05	1 1146 510
2984	36	9.65e-02,	3.57e-03	1.91e-06	1 1656 737
3721	36	7.95e-02,	3.24e-03	1.90e-06	1 2065 919
4640	41	7.46e-02,	2.27e-03	9.47e-07	1 2575 1146
6705	72	9.46e-02,	8.82e-04	1.19e-07	1 3721 1656
8361	82	8.86e-02,	6.78e-04	7.50e-08	1 4640 2065
12082	123	9.57e-02,	3.26e-04	1.67e-08	1 6705 2984
15066	162	1.03e-01,	2.02e-04	5.71e-09	1 8361 3721
18787	198	1.04e-01,	1.33e-04	2.45e-09	1 10426 4640
27148	287	1.08e-01,	6.86e-05	5.97e-10	1 15066 6705
33853	360	1.11e-01,	4.67e-05	2.37e-10	1 18787 8361
42214	450	1.14e-01,	3.08e-05	1.05e-10	1 23427 10426
61001	648	1.17e-01,	1.61e-05	2.44e-11	1 33853 15066
76067	810	1.20e-01,	1.06e-05	9.95e-12	1 42214 18787
94854	1008	1.22e-01,	8.15e-06	5.55e-12	1 52640 23427
137068	1086	9.37e-02,	5.89e-06	2.50e-12	1 76067 33853
170921	1086	7.66e-02,	4.62e-06	1.96e-12	1 94854 42214
246988	2628	1.32e-01,	1.35e-06	1.11e-13	1 137068 61001
384056	2438	8.16e-02,	1.11e-06	3.44e-14	1 213135 94854
554977	5130	1.22e-01,	4.27e-07	6.20e-14	1 307989 137068
862966	6759	1.07e-01,	2.21e-07	4.22e-15	1 478910 213135

TABLE 6.3. Best ρ three-dimensional rules induced by Szekeres 2-fractions with elements bounded by $M = 2$ and order not exceeding 1000. Entries for which the value of N appears with an asterisk describe rules which are best ρ with respect to the set of rank 1 simple three-dimensional rules.

N	ρ	z_s	P_2	P_4	\mathbf{g}
9	2	4.88e-01	6.97e+00	8.80e-01	1 5 2
21 *	3	4.35e-01	2.33e+00	1.17e-01	1 13 3
30	4	4.53e-01	1.39e+00	3.62e-02	1 16 9
41	5	4.53e-01	8.77e-01	1.40e-02	1 22 13
47	6	4.92e-01	7.13e-01	9.14e-03	1 25 9
66 *	8	5.08e-01	4.29e-01	2.94e-03	1 43 9
89	9	4.54e-01	2.81e-01	1.39e-03	1 53 23
101	10	4.57e-01	2.33e-01	9.85e-04	1 61 26
111	12	5.09e-01	1.98e-01	6.53e-04	1 61 35
136	13	4.70e-01	1.48e-01	3.76e-04	1 81 35
153	15	4.93e-01	1.19e-01	2.19e-04	1 97 23
167	16	4.90e-01	1.03e-01	1.56e-04	1 106 25
183	18	5.12e-01	8.90e-02	1.12e-04	1 119 25
231	20	4.71e-01	6.42e-02	7.30e-05	1 121 47
241	21	4.78e-01	5.63e-02	4.39e-05	1 142 63
273	26	5.34e-01	4.73e-02	3.15e-05	1 150 86
327	28	4.96e-01	3.52e-02	1.77e-05	1 185 79
374	30	4.75e-01	2.84e-02	1.24e-05	1 195 77
375	32	5.06e-01	2.78e-02	1.01e-05	1 238 56
419	33	4.76e-01	2.48e-02	9.70e-06	1 243 98
422	34	4.87e-01	2.40e-02	8.99e-06	1 255 109
426	35	4.97e-01	2.32e-02	8.08e-06	1 257 49
466	36	4.75e-01	2.07e-02	6.82e-06	1 302 91
469	40	5.25e-01	1.95e-02	5.42e-06	1 283 54
512	42	5.12e-01	1.70e-02	4.29e-06	1 309 59
543	48	5.57e-01	1.45e-02	2.22e-06	1 320 142
613	51	5.34e-01	1.25e-02	2.02e-06	1 337 193
650 *	57	5.68e-01	1.09e-02	1.35e-06	1 383 170
737 *	64	5.73e-01	8.71e-03	8.00e-07	1 417 178
809	65	5.38e-01	8.17e-03	8.91e-07	1 488 93
882 *	76	5.84e-01	6.58e-03	4.80e-07	1 499 213
919	80	5.94e-01	6.09e-03	3.79e-07	1 520 222
979	81	5.70e-01	5.55e-03	3.18e-07	1 577 256

however, the complexity of enumerating all candidate $(s - 1)$ -fractions of length k , say, is exponential in k —the number of such fractions is 2^k . Thus, large-scale search procedures such as that used to generate Table 6.3 are infeasible for high-order rules. However, smaller-scale searches over sample sets of $(s - 1)$ -fractions with elements subject to such bounds are feasible. Tables A.7–A.12 of the Appendix contain the results of searches in three ‘windows’—similar to those used by Sloan and Walsh [42] and Disney and Sloan [11]—over a set of $(s - 1)$ -fractions. These

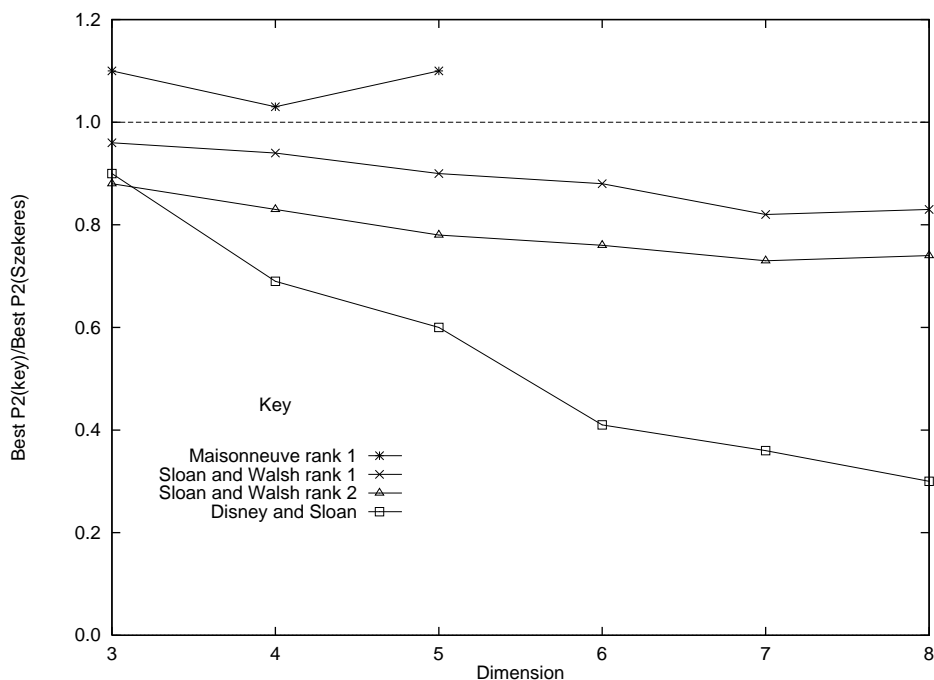


FIGURE 6.1. Ratios of best P_2 values obtained in the 1000-point window

searches were conducted on a Silicon Graphics workstation running Unix System V.3. The sample sets of $(s-1)$ -fractions were generated as follows: for each fraction, the upper bound $M \in \{2, 3\}$ was chosen, using the system pseudorandom number generator. Each integer in the set $R = \{1, \dots, M\}$ was then assigned an integer weight, also in R , again using the system pseudorandom number generator. Finally, the elements of the $(s-1)$ -fraction were chosen from R according to the probability distribution determined by the set of weights. Figures 6.1–6.3 present a comparison in each window, in dimensions 3 to 8, of the ratios of the best P_2 error obtained by the use of Szekeres $(s-1)$ -fractions with those reported for Korobov-type rank-1 rules in Tables 1–6 of Maisonneuve [28], those obtained in the searches by Sloan and Walsh of rank-1 simple rules and rank-2 Korobov-type rules with $n = 2$ (in their terminology), and those obtained in the maximal-rank searches of Disney and Sloan.

When interpreting Figures 6.1–6.3, it should be noted that the numbers of rules considered in each search window are not the same for each of the search procedures. The windows used were: $948 \leq N \leq 1052$ (the 1000-point window), $9972 \leq N \leq 10764$ (the 10000-point window) and $99500 \leq N \leq 100500$ (the 100000-point window). In each of the three windows, Disney and Sloan consider at most 50 rules in each dimension. On the other hand, in the 1000-point window Sloan and Walsh consider 14 values of N and, for each value, N values of $\hat{\mathbf{g}}$ in their search of rank-1 simple Korobov-type rules for comparison with rank-2 rules having $n = 2$. In their searches for rules of the latter type, they consider 5239 rules in \mathbb{R}^3 , 10458 in \mathbb{R}^4 , 17430 in \mathbb{R}^5 , 27888 in \mathbb{R}^6 , 40089 in \mathbb{R}^7 and 55776 in \mathbb{R}^8 . In the 10000-point window, for each dimension, Sloan and Walsh consider 10364 rules in

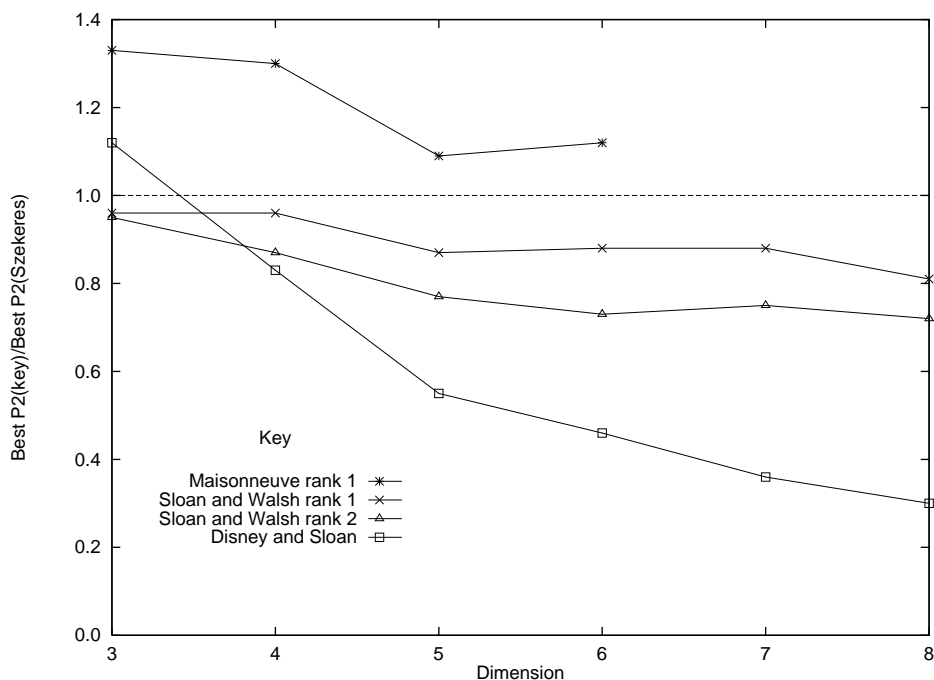


FIGURE 6.2. Ratios of best P_2 values obtained in the 10000-point window

their ‘reduced’ rank-2 search with $n = 2$, and 41472 rank-1 simple rules. In the 100000-point window Sloan and Walsh conducted only reduced searches for rank-2 rules with $n = 2$, for a single value of N in each dimension. The searches in \mathbb{R}^3 to \mathbb{R}^5 were conducted over samples of 1250 and 125 rules. Those in \mathbb{R}^6 to \mathbb{R}^8 were all conducted over samples of 125 rules.

Sloan and Walsh [42, §5] report that their best rank-2 rules with $n = 2$ generally perform better than their best rank-1 rules and rank-2 rules with $n = 3$. In the 1000-point window they report [42, p. 293], a slight predominance of Korobov-type rank-2 rules amongst the best rank-2 rules with $n = 2$. For these reasons the present author conducted searches over samples of the same sizes as those used by Sloan and Walsh in the case of rank-2 Korobov-type rules with $n = 2$.

Figure 6.1 indicates that our best P_2 rules are, in the 1000-point window, consistently better than those reported by Maisonneuve [28], as indicated by a ratio exceeding one. However, they are, at best, slightly inferior to those found by the methods of Sloan and Walsh [42] and Disney and Sloan [11], and this comparison becomes much less favorable as the dimension increases, particularly with respect to the results of Disney and Sloan. Figure 6.2 indicates that, in the 10000-point window, our results are again consistently better than those reported by Maisonneuve and that, at least in dimension three, they are at least comparable with those of Disney and Sloan and the rank-1 results of Sloan and Walsh. Again, this comparison with the higher-rank rules becomes less favorable as the dimension increases. Figure 6.3 shows that, in the 100000-point window, our results are again better with respect to P_2 than those presented in Maisonneuve, except in dimension 8. Furthermore, our results are now at least comparable with those of both Sloan and

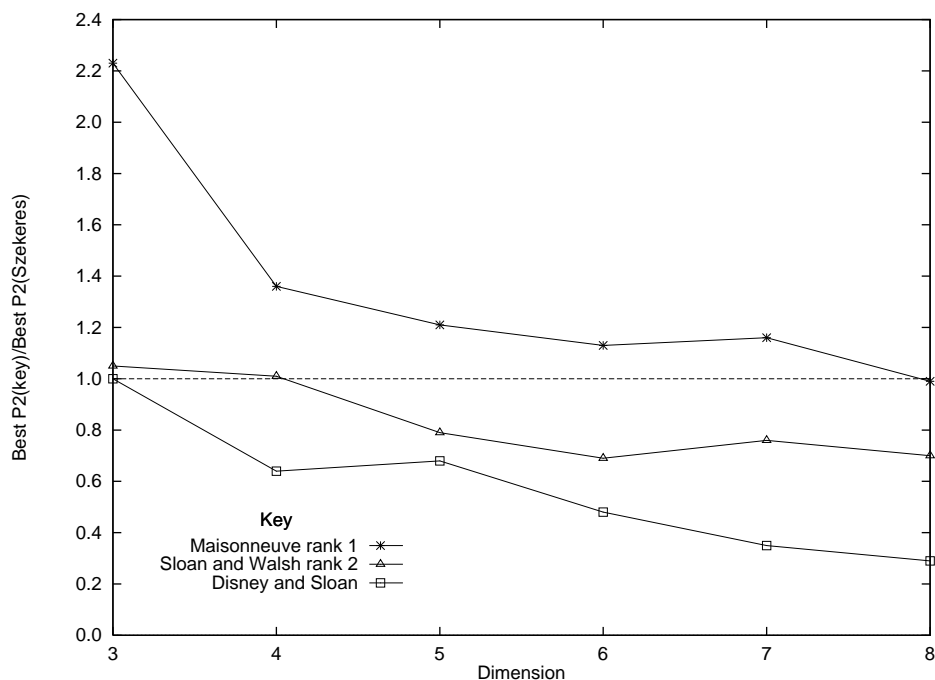


FIGURE 6.3. Ratios of best P_2 values obtained in the 100000-point window

Walsh (rank-2 rules only—no rank-1 data are available) and Disney and Sloan in dimension three, and with those of Sloan and Walsh in dimension four. Again, the comparison deteriorates markedly as the dimension increases.

7. CONCLUDING REMARKS

In this paper we have suggested a connection between badly approximable vectors and lattice rules. Further, we have shown that a technique originating in the theory of simultaneous Diophantine approximation may be adapted to provide a convenient method for constructing rank-1 simple lattice rules, and that the best rules so constructed compare, for low dimensions, not unfavorably with those that have been obtained by other authors. The numerical results described in §6 corroborate the theoretical results of Disney and Sloan [11] and Joe and Disney [16], which indicate that certain maximal-rank rules may be competitive with rules of lower rank but comparable order.

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