A Search for Good Lattice Rules Based on the Reciprocal Lattice Generator Matrix*

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Abstract

The search for cost-effective lattice rules is a time-consuming and difficult process. After a brief overview of some of the lattice theory relevant to these rules, a new approach to this search is suggested. This approach is based on a classification of lattice rules using "the upper triangular lattice form" of the reciprocal lattice generator matrix.

1 Background

A lattice rule is a numerical quadrature rule for integrating over an s-dimensional hypercube. It is a generalization of the one-dimensional trapezoidal rule using a subset of the nodes that would be used by the Cartesian product trapezoidal rule. Number theoretic rules, associated with Korobov (1959), Hwalka (1962), and Niederreiter (1988) form a major subset of the set of lattice rules.

Since their inception, several large-scale searches for good number theoretic rules have been reported in the open literature. Among the most successful are those of Maisonneuve (1972), Kedem and Zaremba (1974), and Bourdeau and Pitre (1985). The number of potential candidates is vast and the construction and organization of these searches has proved to be a challenging task. Using the most up to date computers available, scientists have taken advantage of every available mathematical property to streamline their program.

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In this paper we draw attention to a particular form of the generator matrix of the reciprocal lattice. While this form has proved to be useful in the general theory of lattice rules, here we emphasize only its use as the basis for a search which includes all lattice rules.

We begin by describing some of the underlying theory; in Section 1 we define lattices, lattice rules, and the reciprocal lattice. In Section 2, we introduce the upper triangular lattice form of its generator matrix and propose that this be used to classify lattice rules. In Section 3, the relation between the discretization error in terms of Fourier coefficients and the reciprocal lattice is briefly reviewed; and a standard criterion for assessing the quality of a rule is described. In Section 4, searches for "good" rules are put into perspective and some preliminary results, based on a pilot version of our search, are presented.

Without loss of generality, we treat quadrature over the s-dimensional unit hypercube $[0,1)^s$. In the sequel, all vectors are s-dimensional having rational elements. In particular, $\mathbf{e}_j$ denotes the j-th unit vector (whose components coincide with those of the j-th row of the $s \times s$ unit matrix I).

DEFINITION 1.1. *The unit lattice Λ_0 comprises all points $\boldsymbol{\lambda} = (\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(s)})$ all of whose components $\lambda^{(i)}$ are integers.*

This familiar array of points is the most fundamental lattice. A general definition follows.

DEFINITION 1.2. *A set of points form a lattice Λ when*

$$\mathbf{p}, \mathbf{q} \in \Lambda \Rightarrow \mathbf{p}+\mathbf{q},\ \mathbf{p}-\mathbf{q} \in \Lambda$$

and there exists ε such that

$$\mathbf{p} \neq \mathbf{q} \Rightarrow |\mathbf{p}-\mathbf{q}| \geq \varepsilon .$$

Given $\mathbf{c}_i$, $i=1,2,\ldots,u$, the set of points

$$\mathbf{p} = \Sigma \lambda^{(i)} \mathbf{c}_i \quad \forall \text{ integer } \lambda^{(i)} \tag{1.3}$$

clearly form a lattice. Here, the vectors $\mathbf{c}_i$ are known as *generators*. The same s-dimensional lattice Λ may be generated in many ways, but does not *require* more than s generators. These may be assembled in an $s \times s$ matrix A. Then (1.3) takes the form

$$\mathbf{p} = \boldsymbol{\lambda} A \quad \forall\ \boldsymbol{\lambda} \in \Lambda_0 . \tag{1.4}$$

The matrix A is termed a generator matrix of Λ, and its rows $\mathbf{a}_r$ are, of course, a set of generators of Λ. When $\det A \neq 0$, these are linearly independent and are collectively known as a *basis* for Λ.

The lattice rule $Q(\Lambda)$ is constructed using an *integration lattice.*

DEFINITION 1.5. *An integration lattice Λ is one that contains Λ_0 as a sublattice.*

Given $\mathbf{z}_i \in \Lambda_0$ and integers n_i and t, it is clear that the points

$$\mathbf{p} = \sum_{i=1}^{t} j_i \mathbf{z}_i / n_i + \sum_{i=1}^{s} \mu^{(i)} \mathbf{e}_i \quad \forall \text{ integer } j_i \text{ and } \boldsymbol{\mu} \in \Lambda_0 \tag{1.5}$$

form an integration lattice. Note that an integration lattice Λ satisfies

$$d^{-1}\Lambda_0 \supseteq \Lambda \supseteq \Lambda_0 \tag{1.6}$$

for some integer d.

DEFINITION 1.7. *The lattice rule $Q(\Lambda)$ defined when Λ is an integration lattice is one that assigns an equal weight N^{-1} to every point*

$$\mathbf{p} \in \Lambda \cap [0,1)^s .$$

When Λ is given by (1.5), this lattice rule may be written as

$$Q(\Lambda)f = \frac{1}{n_1 n_2 \ldots n_t} \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \cdots \sum_{j_t=1}^{n_t} \bar{f}\left[\sum_{i=1}^{t} j_i \mathbf{z}_i / n_i \right] . \tag{1.8}$$

Here $\bar{f}(\mathbf{x})$ is a periodically continued version of $f(\mathbf{x})$ that coincides with $f(\{\mathbf{x}\})$ when $\{\mathbf{x}\} \in (0,1)^s$. For details, see Lyness (1989). Expression (1.8) is termed a t-cycle form of the lattice rule. It is not unique, and may be repetitive (i.e. include each point k times). One can always express a rule in this form with $t \leq s$. The *rank* r of a rule is the smallest value of t for which it may be written in this form. Thus a rule of rank 1

$$Qf = \frac{1}{N} \sum_{j=1}^{N} \bar{f}(j\mathbf{z}/N) \tag{1.9}$$

coincides with the number theoretic rule of Korobov. The joint publications of Sloan and Lyness in 1989 and 1990 are devoted to obtaining properties of lattice rules based almost exclusively on this definition. Exploiting finite Abelian group theory, we have made significant headway in classifying lattice rules. However, many problems remain unresolved.

A fundamental concept in lattice theory is the reciprocal lattice or polar lattice (denoted by $\Lambda^\perp$) of a lattice Λ.

DEFINITION 1.10. *The reciprocal lattice of Λ, denoted by $\Lambda^\perp$, comprises all $\mathbf{r}$ such that*

$$\mathbf{p} \cdot \mathbf{r} = \text{integer} \quad \forall\ \mathbf{p} \in \Lambda .$$

It can be shown that when A is a generator matrix of Λ, then $B = (A^T)^{-1}$ is a generator matrix of $\Lambda^\perp$. The reciprocal lattice $\Lambda^\perp$ occurs naturally in expansion (3.1) below for the discretization error. However, it also provides a simple criterion for whether the lattice Λ defined in terms of A is an integration lattice, i.e., $\Lambda \supseteq \Lambda_0$.

THEOREM 1.11. *Λ is an integration matrix if and only if any generator matrix B of $\Lambda^{\perp}$ is an integer matrix, i.e., all its elements are integers.*

It can be shown that when Λ is an integration matrix, and $B = (A^T)^{-1}$,

$$N = |\det A|^{-1} = |\det B| \tag{1.12}$$

is the number of lattice points in $[0,1)^s$, which is, of course, the number of distinct function values $f(\mathbf{x})$ required by the rule $Q(\Lambda)$. Moreover, it is the smallest value of d for which (1.6) is valid and

$$N\Lambda_0 \subseteq \Lambda^{\perp} \subseteq \Lambda_0 \, . \tag{1.13}$$

2 The Upper Triangular Lattice Form (utlf) of B

A pervasive source of difficulty in all these results is the extreme lack of uniqueness. The same lattice Λ may be defined by using many different sets of generators in (1.3), (1.4), or (1.5) and the same rule may be defined by using different $\mathbf{z}_i, n_i$ in (1.8) or (1.9) even when t coincides with the rank of $Q(\Lambda)$. Much of the work based on (1.8) has been in search of uniqueness. So far as generator matrices A or B are concerned, it is almost self-evident that adding one row to another while altering the matrix has no effect on the lattice Λ. The same lattice Λ is now described using a different set of generators. Such an integer row operation may be described in terms of pre-multiplication by a unimodular matrix U. This is an integer matrix having $|\det U| = 1$. Thus, B and UB generate the same lattice so long as U is unimodular. This may be exploited to transform B into *upper triangular lattice form* defined below; we find there is a (1-1) correspondence between each distinct integer matrix of this form and each distinct integer lattice $\Lambda^{\perp}$.

DEFINITION 2.1. *An $s \times s$ integer matrix B is of upper triangular lattice form (utlf) if and only if*

(a) All elements below the diagonal are zero, i.e.,

$$b_{r,c} = 0 \quad r > c \, ;$$

(b) All diagonal elements are positive integers, i.e.,

$$b_{c,c} \geq 1 \, ;$$

(c) All elements are nonnegative, and the unique maximum element in any column is the diagonal element, i.e.,

$$0 \leq b_{r,c} < b_{c,c} \quad r = 1,2,,\ldots,s \, .$$

The principal theorem of this paper follows.

THEOREM 2.2. *Every integer lattice Λ has one and only one generating matrix B of upper triangular lattice form.*

A version of this theorem is given in Cassells (1959), Section I.2.2. As it applies to integer matrices, this result is classical and the utlf is essentially the Hermite Normal Form. An excellent description of this part of elementary lattice theory is given in Section 4 of Schrijver (1986). A useful discussion and algorithm is given in G. Bradley (1971).

This classification is dealt with in considerable detail in an ANL report, Lyness and Newman (1989), which is a preliminary and extended version of the present article. In particular, a straightforward triangularization algorithm is described. Other relations between the utlf of B and the lattice rule with which it is associated are given. And attention is drawn to a major drawback to classification using the generator matrix A of Λ directly.

We have found the utlf of B useful also in developing the general theory of lattice rules. See, for example, Lyness and Sørevik (1989) and Lyness, Sørevik, and Keast (1990). In this article we treat only the application to the search.

3 The Good Lattices

The error made by any quadrature rule may be expressed in terms of the s-dimensional Fourier coefficients $a_{\mathbf{m}}$ of the integrand function using a generalization of the Poisson Summation Formula. (This is the basis of much of the theory of number theoretic rules. A discussion in the context of lattice rules appears in Lyness (1988).) For lattice rules $Q(\Lambda)$, it can be shown that the Poisson Summation Formula reduces to

$$Q(\Lambda)\bar{f} - I\bar{f} = \sum_{\substack{\mathbf{m}\in\Lambda^{\perp} \\ \mathbf{m}\neq\mathbf{0}}} a_{\mathbf{m}} . \tag{3.1}$$

Here $a_{\mathbf{m}}$ is the multivariate Fourier coefficient and $\Lambda^{\perp}$ is the reciprocal lattice of the lattice Λ on which the rule is based. This suggests a criterion for choosing from the many available N-point lattice rules those that may be cost effective. Specifically, one chooses Λ so that the larger Fourier coefficients on the right drop out. Before we are able to apply this, we have to decide which are the more significant Fourier coefficients. This issue is discussed in detail in Lyness (1988). The conventional wisdom is to proceed as follows. Let

$$\rho(\mathbf{m}) = \rho(m_1, m_2, \ldots, m_s) = \prod_{i=1}^{s} \max(|m_i|, 1) \qquad \mathbf{m} \in \Lambda_0 ;$$

then define the Zaremba rho-index of an integer lattice by

$$\rho(\Lambda^{\perp}) = \min_{\substack{\mathbf{m}\in\Lambda^{\perp} \\ \mathbf{m}\neq\mathbf{0}}} \rho(\mathbf{m}) .$$

The "good" lattice rules $Q(\Lambda)$ are those for which $\rho(\Lambda^{\perp})$ is largest.

4 Some New Lattice Rules

The theory of this paper may be used to construct a search program to find cost-effective lattice rules. Previous searches for "good lattice rules" are described by Maisonneuve (1972), Kedem and Zaremba (1974), and Bourdeau and Pitre (1985). Between them, these authors have considered number theoretic rules in dimensions $s = 3$, 4, and 5 with N up to $N = 6066$, 3298, and 772, respectively. They have demonstrated that a clear appreciation of the problem and sophisticated coding technique can lead to significant economy and speedup. All these searches, of course, were confined to number theoretic rules which are of form (1.9) above and were based on treating in turn different parameters $\mathbf{z}$ for given values of s and N.

On the other hand, we have used Theorem 2.2 above as the basis for an exhaustive search for cost effective lattice rules. For given values of s and N, such a program employs an outer loop in which all sets of positive integers $v_1, v_2, \dots, v_s$ for which $v_1 v_2 \cdots v_s = N$ are included. Then for a given set $v_1, v_2, \dots, v_s$, all combinations of off-diagonal elements $b_{r,c}$ $r = 1,2,\dots,s-1$; $c = 2,3,\dots,s$ are treated for which

$$0 \le b_{r,c} < v_c \ .$$

We expect that the organization of such a search, and the number of distinct lattice rules $v_s(N)$, will form the topics of other articles (Lyness and Sørevik (1989)).

In this search, as in the other searches, a critical feature concerns the possibility of avoiding separate treatment of different lattices that are related by affine transformation. In the various search procedures we have encountered, this is handled in a somewhat *ad hoc* manner, which relies partly on theory and partly on inelegant and sometimes cumbersome algorithms. The present search is no exception in this respect. It seems to be just as bad or good as the previous searches. It is this sort of theoretically peripheral but practically vital circumstance on which an ultimate choice of methods is likely to depend.

At this point we have carried out only a primitive search, as a pilot scheme, with $s = 3$ and $N < 150$. Even this limited search has uncovered new rules, mainly of academic interest. The list in Table 1 gives the additional entries required to extend Maisonneuve's list to include all lattice rules, following the convention introduced by her for listing these rules. That is, one includes a rule if there is no rule having a smaller value of N and the same value of ρ; but one does not include rules that can be obtained from rules already on the list by an affine transformation of the cube into itself.

Table 1. Some New Three-Dimensional Lattice Rules

N	ρ	n_1	$\mathbf{z}_1$	n_2	$\mathbf{z}_2$	n_3	$\mathbf{z}_3$
16	4	4	(1,1,1)	2	(0,1,0)	2	(0,0,1)
42	6	42	(2,3,16)				
54	8	18	(1,2,10)	3	(0,1,0)		
54	8	18	(1,5,5)	3	(0,1,2)		
96	12	48	(3,9,28)	2	(0,1,0)		
144	16	36	(1,11,5)	2	(0,1,0)	2	(0,0,1)

These rules are given in the canonical form of Sloan and Lyness (1989), specifically

$$Qf = \frac{1}{n_1 n_2 n_3} \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \sum_{j_3=1}^{n_3} \bar{f}\left\{ \frac{j_1 \mathbf{z}_1}{n_1} + \frac{j_2 \mathbf{z}_2}{n_2} + \frac{j_3 \mathbf{z}_3}{n_3} \right\},$$

where n_i divides n_{i-1} and $N = n_1 n_2 n_3$. We note that rules of ranks 1, 2, and 3 appear. Those of rank 3 are 2^3–copy versions of lattice rules having $N/8$ abscissas.

The 42-point rule is interesting because it is a rank 1 (number theoretic) rule, which was not discovered by Maisonneuve. Her search omits a relatively small class of number theoretic rules that can be expressed in number theoretic form (1.9) only with all components of $\mathbf{z}_1$ greater than unity.

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