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A CLASSIFICATION OF LATTICE RULES USING THE RECIPROCAL LATTICE GENERATOR MATRIX

by

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Mathematics and Computer Science Division

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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), Hwarka (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.

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 that includes all lattice rules.

We begin by describing some of the underlying theory; we define lattices, lattice rules, and the reciprocal lattice. In Section 2, we introduce the upper triangular lattice form (utlf) 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 $\boldsymbol{\lambda} = (\lambda^{(1)}, \lambda^{(2)}, \dots, \lambda^{(s)})$ all of whose components $\lambda^{(i)}$ are integers.*

This familiar array of points is the most fundamental lattice. A more 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 $\varepsilon > 0$ such that

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

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

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

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

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

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

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

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

$$d^{-1} \Lambda_0 \supseteq \Lambda \supseteq \Lambda_0 \quad (1.6)$$

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

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

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

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

coincides with the number theoretic rule of Korobov. The joint publications of Sloan and Lyness (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. $\Lambda^\perp$ 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 $B = (A^T)^{-1}$,

$$N = |\det A|^{-1} = |\det B| \quad (1.12)$$

is the number of lattice points in $[0, 1)^s$, which is, of course, the number of distinct function

values $\bar{f}(\mathbf{x})$ required by the rule $Q(\Lambda)$. Moreover, it is the smallest value of d for which (1.6) is valid and

$$N\Lambda_0 \subseteq \Lambda^\perp \subseteq \Lambda_0. \quad (1.13)$$

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 r 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 well known (Cassels 1959, Chapter I) that B and TB generate the same lattice provided T is an integer matrix and $|\det T| = 1$. When this fact is 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.,*

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

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 Cassels (1959), Section I.2.2. It is well known that one may carry out elementary integer row operations on any generating matrix B without altering the lattice Λ . One may use these to transform B (which we recall is nonsingular) into upper triangular form. Either after this is done or during the process, it is straightforward to arrange that the superdiagonal elements satisfy condition (c). In Appendix A, a triangularization algorithm is

described that accomplishes this task. The other appendixes give other connections between the utlf of B and the lattice rule with which it is associated. The difficulty involved when using the generator matrix A of Λ directly is touched on in Appendix E.

We have found the utlf of B useful also in developing the theory of lattice rules. See, for example, Lyness and Sørveik (1989) and Lyness, Sørveik, and Keast (1988). 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

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

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

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

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

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

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 Srevik 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 in practice 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	(3,4,2)				
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

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

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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Appendix A: The Algorithm

In this appendix, we describe an algorithm that transforms a nonsingular $s \times s$ matrix B having integer elements to one of "upper triangular lattice form" using only the elementary row operations

$$\mathbf{b}'_r = -\mathbf{b}_r \quad (\text{A.1})$$

$$\mathbf{b}'_r = \mathbf{b}_r + \lambda \mathbf{b}_s, \quad \lambda \text{ integer } s \neq r \quad (\text{A.2})$$

and (the row interchange operation)

$$\mathbf{b}'_r = \mathbf{b}_s; \quad \mathbf{b}'_s = \mathbf{b}_r \quad (\text{A.3})$$

Note that the magnitude of determinant $|\det B|$ is unaltered by any of these operations.

Our algorithm involves s major stages, each dealing with one column. We now describe in detail stage j .

At the beginning of stage j , B satisfies

$$b_{i,k} \text{ integer and } \det B \neq 0 \quad (\text{A.4})$$

$$b_{i,i} > 0 \quad i = 1, 2, \dots, j-1 \quad (\text{A.5})$$

$$0 \leq b_{r,c} < b_{c,c} \quad r < c \quad c = 1, 2, \dots, j-1 \quad (\text{A.6})$$

$$b_{r,c} = 0 \quad r > c \quad c = 1, 2, \dots, j-1. \quad (\text{A.7})$$

At the end of stage j , B satisfies the same relations with $j-1$ replaced by j , and so is ready for stage $j+1$. Stage j is in four parts. Parts 1, 2, and 3 deal only with the elements in rows $j, j+1, \dots, s$. We recall that at the start of stage j , each of these rows has zero in positions $1, 2, \dots, j-1$. Thus any transformation involving only these rows leaves zero in these early positions. The purpose of these parts is to carry out row operations that, respectively,

- (1) Replace the set of elements

$$C_j^L = (b_{j,j}, b_{j+1,j}, \dots, b_{s,j})$$

by a set in which each element is nonnegative.

- (2) Replace the set C_j^L by a set that contains only one positive element, all the rest being zero.
- (3) Replaces this set by one in which $b_{j,j} \neq 0$ but all other elements are zero.

The final part does not involve altering any of the rows $j, j+1, \dots, j+s$.

- (4) Replace the set of elements

$$C_j^U = (b_{1,j}, b_{2,j}, \dots, b_{j-1,j})$$

by a set in which each element lies in range $[0, b_{j,j})$.

Parts 1, 3, and 4 are trivial. Part 1 is accomplished by using (A.1) to replace $\mathbf{b}_r$ by $-\mathbf{b}_r$ for those values of r in $[j, s]$ for which $b_{r,j}$ is negative. Part 3 is accomplished by using (A.3) to interchange the single row r in $[j, s]$ for which $b_{r,j} \neq 0$ with row j . Part 4 is accomplished by using (A.2);

$$\mathbf{b}'_r = \mathbf{b}_r - \lfloor b_{r,j}/b_{j,j} \rfloor \mathbf{b}_j \quad r = 1, 2, \dots, j-1,$$

where $\lfloor x \rfloor$ denotes the integer part (floor) of x .

Part 2 is more interesting. One method of finding the h.c.f. of a set of nonnegative integers is the following: if any two are nonzero, subtract the smaller from the larger (or from one the same size). This may always be done when there are two or more nonzero elements. The elements remain nonnegative but their sum reduces. This process, applied to the set $(b_{j,j}, \dots, b_{s,j})$, may be continued until the set is replaced by $(0, 0, \dots, 0, v_j, 0, \dots, 0)$. The second part of this stage of the algorithm consists of carrying out precisely this process, but, of course, dealing with the entire row rather than just the first nonzero element. Thus one carries out a sequence of operations

$$\mathbf{b}'_r = \mathbf{b}_r - \mathbf{b}_s \quad r, s \leq j \quad (b_{r,j} \geq b_{s,j})$$

until there is only one row, say the k -th, which has a nonzero j -th component. This concludes our description of stage j .

The algorithm to put B in upper diagonal lattice form involves carrying out successively stages $1, 2, \dots, s$. Prior to stage 1, there are no restrictions on the elements $b_{i,j}$ other than that the elements be integer and that $\det B \neq 0$. None of the operations in any stage alter these properties. At the end of stage j , B satisfies the initial conditions for stage $j+1$. And the final conditions of stage s , obtained by setting $j = s$ in (A.4)-(A.7), coincide with the Definition 2.1.

We note that stage 1 does not require a part 4 (since C_1^U is empty) while stage s does not require parts 2 and 3 (since C_s^L contains a single element).

We also note that part 4 of any stage may be delayed and is not needed to carry out parts 1, 2, and 3 of later stages. However, part 4 of stage j cannot be usefully carried out until part 4 of the previous stages has been carried out in order.

By definition, every integer lattice has a generator matrix B . Using the preceding algorithm, we may transform B to be of upper triangular lattice form. Thus every integer lattice has a generator matrix of this form. The principal remaining question in this article is whether this form is unique. In fact, it is unique. This will be established in Appendix C. That proof is not the most direct, but exploits an interesting geometric interpretation of the diagonal elements introduced in Appendix B.

Appendix B: Projections

It is convenient to introduce the Cartesian projections of an s -dimensional lattice $\Lambda^{(s)}$. The principal s' -dimensional projection $\Lambda^{(s')}$, with $s' \leq s$, is defined by

$$\mathbf{p} = (p_1, p_2, \dots, p_{s'}) \in \Lambda^{(s')}$$

if and only if there exists $p_{s'+1}, \dots, p_s$ such that

$$\mathbf{r} = (p_1, p_2, \dots, p_{s'}, p_{s'+1}, \dots, p_s) \in \Lambda^{(s)}.$$

It is elementary to verify that when $\Lambda^{(s)}$ is an integration lattice or an integer lattice, $\Lambda^{(s')}$ has the same character.

Other s' -dimensional projections are defined in a similar way in terms of a specified s' -dimensional subspace. That is, let $i_1, i_2, \dots, i_{s'}$ be a permutation of $1, 2, \dots, s$. Then $\tilde{\Lambda}^{(s')}$ defined by

$$\mathbf{p} = (p_{i_1}, p_{i_2}, \dots, p_{i_{s'}}) \in \tilde{\Lambda}^{(s')}$$

if and only if for some $p_{i_{s'+1}}, \dots, p_{i_s}$,

$$\mathbf{r} = (p_1, p_2, \dots, p_s) \in \Lambda^{(s)}$$

is termed a projection of $\Lambda^{(s)}$ into the s' -dimensional $x^{i_1}, x^{i_2}, \dots, x^{i_{s'}}$ manifold.

We shall use the following self-evident proposition. Let $\Lambda_1^{(s)}$ and $\Lambda_2^{(s)}$ be s -dimensional lattices whose principal s' -dimensional projections with $s' < s$ are $\Lambda_1^{(s')}$ and $\Lambda_2^{(s')}$, respectively. If $\Lambda_1^{(s')} \neq \Lambda_2^{(s')}$, then $\Lambda_1^{(s)} \neq \Lambda_2^{(s)}$.

Note that the converse is not generally true.

THEOREM B.1. *Let B be an upper triangular generating matrix of the s -dimensional integer lattice $\Lambda^{(s)}$. Then $\tilde{B}$, the $s' \times s'$ principal minor of B , is an upper triangular generating matrix for the s' -dimensional principal projection $\Lambda^{(s')}$ of $\Lambda^{(s)}$.*

Note that if B is in upper triangular lattice form, so is $\tilde{B}$.

Proof. By definition, the elements of $\Lambda^{(s)}$ are of the form

$$\mathbf{r} = \sum_{j=1}^s \lambda_j (b_{j,1}, b_{j,2}, \dots, b_{j,s}).$$

It follows from the definition that the elements of $\Lambda^{(s')}$ are of the form

$$\mathbf{p} = \sum_{j=1}^s \lambda_j (b_{j,1}, b_{j,2}, \dots, b_{j,s'}).$$

Since the matrix B is upper triangular, the final $s-s'$ elements $\mathbf{b}_j$ are each zero vectors and may

be omitted from the sum. Thus the general element of $\Lambda^{(s')}$ is

$$\mathbf{p} = \sum_{j=1}^{s'} \lambda_j(b_{j,1}, b_{j,2}, \dots, b_{j,s'})$$

and is of the form $\mathbf{p} = \lambda \tilde{B}$ where $\tilde{B}$ is the principal $s' \times s'$ minor of B . $\square$

We recall that the inverse point density of the lattice Λ is given by $|\det B| = (v_1 v_2 \cdots v_s)$. The principal projections $\Lambda^{(t-1)}$ and $\Lambda^{(t)}$ have the corresponding principal minors of B as generating functions. This fact leads immediately to the following corollary.

COROLLARY. *The t -th diagonal element v_t of any upper triangular form B of an s -dimensional lattice Λ is the ratio of the point densities of $\Lambda^{(t-1)}$ and $\Lambda^{(t)}$, its principal projections.*

As such, v_t is a constant associated with the lattice Λ . It follows that all upper triangular generator matrices B of a particular lattice have the same diagonal elements. In subsequent papers we shall define the upper class of an s -dimensional lattice Λ as an s -tuple of integers $[v_1, v_2, \dots, v_s]$. Here we simply use the corollary to establish the uniqueness of the upper triangular lattice form.

Appendix C: The Uniqueness of the Representation

THEOREM C.1. *When $B^{(1)}$ and $B^{(2)}$ are both generator matrices of the same integer lattice Λ and both are in upper triangular lattice form, then their elements coincide.*

Proof. The theorem in Appendix B provided a geometric interpretation of the diagonal elements of $B^{(1)}$ or $B^{(2)}$ in terms of Λ . Thus these elements depend only on Λ and not on any particular upper triangular generator matrix. Let column c be the first column in which for some r , say $r = t$, we have

$$b_{t,c}^{(1)} - b_{t,c}^{(2)} \neq 0. \quad (\text{C.2})$$

Thus

$$b_{t,j}^{(1)} = b_{t,j}^{(2)} \quad j = 1, 2, \dots, c-1. \quad (\text{C.3})$$

Let us consider the c -dimensional principal projection $\Lambda^{(c)}$ of Λ . By the theorem of Appendix B, both the principal $c \times c$ minor of $B^{(1)}$ and the corresponding minor of $B^{(2)}$ are equally generator matrices of $\Lambda^{(c)}$. Thus this lattice contains elements $\mathbf{b}_t^{(1)}$ and $\mathbf{b}_t^{(2)}$ (suitably curtailed); and since it is a lattice, it contains

$$\mathbf{b}_t^{(1)} - \mathbf{b}_t^{(2)} = (0, 0, \dots, 0, b_{t,c}^{(1)} - b_{t,c}^{(2)}). \quad (\text{C.4})$$

However, all points of $\Lambda^{(c)}$ are of the form

$$\mathbf{p} = \sum_{r=1}^c \lambda_r \mathbf{b}_r^{(1)}; \quad (\text{C.5})$$

and since $B^{(1)}$ is an upper triangular matrix, the element (C.4) can arise only by setting $\lambda_1 = \lambda_2 = \dots = \lambda_{c-1} = 0$. Since $\mathbf{b}_c^{(1)} = (0, 0, \dots, 0, v_c)$, we find

$$b_{t,c}^{(1)} - b_{t,c}^{(2)} = \lambda_c v_c \quad (\text{C.6})$$

for some integer λ_c . However, by hypothesis, both $B^{(1)}$ and $B^{(2)}$ are matrices of upper triangular lattice form, so both $b_{t,c}^{(1)}$ and $b_{t,c}^{(2)}$ lie in the interval $[0, v_c - 1]$. Their difference then lies in the interval $[-(v_c - 1), (v_c - 1)]$, and so λ_c in (C.6) is zero and $b_{t,c}^{(1)} = b_{t,c}^{(2)}$. This contradicts assertion (C.2), and so invalidates it. Consequently, there is no column c for which some element satisfies (C.2), and the matrices $B^{(1)}$ and $B^{(2)}$ coincide. $\square$

Appendix D: The Lower Triangular Lattice Form

A corresponding classification may be constructed by considering a "lower triangular lattice form" of B . This can be defined as in Section 2 by simply replacing the condition $r > c$ in (a) by $r < c$ and the word "below" by "above". Note that this is not a transpose operation.

In this case the theory is similar to the one described in Appendixes A, B, and C. However, the diagonal elements are quite different; v_t is again the ratio of the point densities of two projections of Λ ; these are $\tilde{\Lambda}^{(t-1)}$ and $\tilde{\Lambda}^{(t)}$ of dimension $t-1$ and t , respectively. $\tilde{\Lambda}^{(t)}$ is the projection of Λ into the space $x^t, x^{t-1}, \dots, x^1$.

We have discovered no obvious connection between the representations of Λ in upper and in lower triangular lattice forms.

Appendix E: The Inverse of B

As mentioned in Section 3, a search through all lattice rules $Q(\Lambda)$ whose abscissa set $A(Q)$ has precisely N elements may be conveniently organized on the basis of the generating matrices B of each reciprocal lattice $\Lambda^\perp$. For many purposes, it is just as convenient to have B readily available rather than, perhaps, A . But should A , the generator matrix of the rule $Q(\Lambda)$, be required, it may be readily evaluated numerically as $A = (B^T)^{-1}$, a particularly concise calculation, as B is already in upper triangular form.

Nevertheless, it is pertinent to see whether such a convenient scheme, based on the generator matrix A itself, exists. To this end we examine the set of lower diagonal matrices $A = (B^T)^{-1}$ which corresponds to the set of matrices B . When B is a 3×3 matrix, we find

$$A = \begin{bmatrix} 1/v_1 & , & 0 & , & 0 \\ -b_{12}/v_1 v_2 & , & 1/v_2 & , & 0 \\ -b_{13}/v_1 v_3 + b_{12}b_{23}/v_1 v_2 v_3 & , & -b_{23}/v_2 v_3 & , & 1/v_3 \end{bmatrix}. \quad (E.1)$$

The structure of the more extreme off-diagonal elements becomes rapidly more complicated with the dimension. In four or more dimensions

$$A_{4,1} = -\frac{b_{14}}{v_1 v_4} + \frac{b_{12}b_{24}}{v_1 v_2 v_4} + \frac{b_{13}b_{34}}{v_1 v_3 v_4} - \frac{b_{12}b_{23}b_{34}}{v_1 v_2 v_3 v_4}.$$

In general, the inverse of B has elements

$$A_{r,r} = 1/v_r$$

$$A_{r,c} = 0 \quad r > c$$

$$A_{r,c} = - \sum_{\mathbf{j} \in S_{c,r}} \frac{b_{r,j_1} b_{j_1,j_2} \cdots b_{j_i,c}}{v_r v_{j_1} v_{j_2} \cdots v_{j_i} v_c} \text{sign}(\mathbf{j}) \quad r < c.$$

The set $S_{c,r}$ contains 2^{r-c-1} elements, these being all generalized integers $\mathbf{j} = (j_1, j_2, \dots, j_i)$ with $c < j_1 < j_2 < \cdots < j_i < r$. The set includes an element $\mathbf{j} = ()$, and associated with each element $\mathbf{j}$ is $\text{sign}(\mathbf{j}) = (-1)^i$ which is ± 1 depending on whether the number of integers in $\mathbf{j}$ is even or odd.

All lattice rules $Q(\Lambda)$ having an abscissa set $A(Q)$ of order N are in (1-1) correspondence with the set of matrices A of the above somewhat complicated form, but constrained by

$$(\det A)^{-1} = N = v_1 v_2 \cdots v_s$$

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

It is clear that the set of matrices A of form (E.1) has a more complicated structure than the corresponding set of reciprocal matrices B ; partly for this reason, our search programs are generally based on matrices B in upper triangular lattice form.

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