

FOUR-DIMENSIONAL LATTICE RULES GENERATED BY SKEW-CIRCULANT MATRICES

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ABSTRACT. We introduce the class of *skew-circulant* lattice rules. These are s -dimensional lattice rules that may be generated by the rows of an $s \times s$ skew-circulant matrix. (This is a minor variant of the familiar circulant matrix.) We present briefly some of the underlying theory of these matrices and rules. We are particularly interested in finding rules of specified trigonometric degree d . We describe some of the results of computer-based searches for optimal four-dimensional skew-circulant rules. Besides determining optimal rules for $\delta = d + 1 \leq 47$, we have constructed an infinite sequence of rules $\hat{Q}(4, \delta)$ that has a limit rho index of $27/34 \approx 0.79$. This index is an efficiency measure, which cannot exceed 1, and is inversely proportional to the abscissa count.

1. INTRODUCTION

This paper is a contribution to the theory of multidimensional cubature over $[0, 1]^s$ of specified *trigonometric* degree d . This work was initiated mainly by Russian authors (for example, [Mys88] and [Nos91]) and has been significantly developed internationally. The extensive introduction of lattice rules (see, for example, [SlJo94]) into this area has broadened the theory. A recent, somewhat detailed, account of some of this work appears in [CoLy01]. Significant computing power (see, for example, [SøMy01]) has been devoted to uncovering new rules.

In this paper, we introduce *skew-circulant* lattice rules. We seek optimal s -dimensional rules of specified *enhanced* degree δ (which is defined as $\delta := d + 1$). We describe a moderate search by means of computer for such rules. New rules in four and three dimensions are presented in Sections 5 and 7.

1.1. Background: Available optimal rules. For a handful of small values of dimension s and enhanced degree δ , *optimal* rules have been known for several years. In particular, optimal rules for all dimensions with $\delta \leq 4$ are known. For $s \geq 4$ no other optimal rules are known. For $s = 3$ an optimal rule for all δ that are multiples of 6 is also available, and for $s = 2$ and trivially for $s = 1$ optimal rules are known for all δ .

Received by the editor October 5, 2001 and, in revised form, May 23, 2002.

2000 *Mathematics Subject Classification.* Primary 65D32; Secondary 42A10.

Key words and phrases. Multidimensional cubature, optimal lattice rules, skew-circulant matrices, K -optimal rules, and optimal trigonometric rules.

This work was supported by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, U.S. Department of Energy, under Contract W-31-109-Eng-38.

It appears that, for each of these (s, δ) values, one or more of the optimal rules is a lattice rule. All of the known optimal lattice rules with $\delta \leq 6$ were discovered or could readily have been discovered by a very limited search (among rank-1 lattice rules only), the optimality being recognized when the abscissa count N coincided with a theoretically established minimum N_{ME} . The others (i.e., $(s, \delta) = (3, 6k); k > 1$) are simply k -copies of the one with $\delta = 6$. To show that these copy rules are optimal requires a simple application of the deeper critical lattice theory of Minkowski [Min11].

During the past ten years, the situation with respect to known optimal rules has not changed significantly. Attention has shifted to treating well-defined subsets of lattice rules and finding, either analytically or by major computer search, optimal rules with respect to this subset. Many apparently excellent lattice rules have been discovered in this way; whether any of these is optimal is not known.

1.2. Lattice rules and their trigonometric degree. An s -dimensional lattice Λ is the set of points generated by all linear integer combinations of s linearly independent vectors \mathbf{a}_j , $j = 1, 2, \dots, s$. These vectors are known collectively as a set of generators of Λ , and a matrix A whose rows comprise these generators in any order is known as a generator matrix for Λ . The unit lattice Λ_0 , also known as $\mathcal{Z}^{(s)}$, is the special lattice comprising all points, all of whose components are integers. It follows that $\mathbf{h} \in \Lambda \Leftrightarrow \mathbf{h} = \lambda A$ for some $\lambda \in \Lambda_0$.

The generator matrix of a lattice is not unique. However, all generator matrices of a particular lattice are related in accordance with the following theorem.

Theorem 1.1. *A and A' are generator matrices of the same lattice if and only if $A = UA'$, where U is a unimodular matrix.¹*

An *integration* lattice Λ is a lattice that satisfies $\Lambda \supseteq \Lambda_0$. An s -dimensional lattice rule $Q(\Lambda)$ is simply an integration rule that applies the same weight $(\nu(\Lambda))^{-1}$ to each of the $\nu(\Lambda)$ points of an s -dimensional integration lattice Λ that lie in $[0, 1]^s$. Thus it integrates a constant function correctly, making it of enhanced degree $\delta(Q) \geq 1$.

Associated with any lattice Λ , generated by A , is its *dual* lattice, Λ^\perp , generated by the matrix $(A^{-1})^T$. A consequence of the fact that for an integration lattice $\Lambda \supseteq \Lambda_0$ is that $\Lambda_0 \supseteq \Lambda^\perp$, which implies that $(A^{-1})^T$ is an *integer* matrix. The dual lattice plays an important role in the theory of lattice rules because it can be used to specify an error expansion of the quadrature rule in terms of the Fourier coefficients, $\hat{f}_{\mathbf{h}}$, of the integrand function as follows:

$$(1) \quad E_{Q(\Lambda)}f = Q(\Lambda)f - If = \sum_{\substack{\mathbf{h} \in \Lambda^\perp \\ \mathbf{h} \neq \mathbf{0}}} \hat{f}_{\mathbf{h}}.$$

Here I is the integration operator over $[0, 1]^s$, and $\hat{f}_{\mathbf{0}} = If$. For a lattice rule to integrate exactly all polynomials of trigonometric degree d , the right-hand side of this equation must vanish whenever f is such a polynomial. This requirement leads to a characterization of the trigonometric degree of a lattice rule² as follows.

¹ A unimodular matrix U is an integer matrix for which $\det(U) = \pm 1$. The inverse of a unimodular matrix is also a unimodular matrix.

²The statement that an integer lattice Λ^\perp is of a specified trigonometric degree d should be taken to mean that the lattice rule $Q(\Lambda)$ is of degree d . The enhanced degree δ is $d + 1$.

Definition 1.2. A lattice rule $Q(\Lambda)$ is of enhanced trigonometric degree δ if and only if $\forall \mathbf{h} \in \Lambda^\perp$, other than $\mathbf{h} = \mathbf{0}$:

$$\|\mathbf{h}\|_1 := |h_1| + |h_2| + \cdots + |h_s| \geq \delta.$$

Definition 1.3. The lattice rule $Q(\Lambda)$ in Definition 1.2 is of *strict* enhanced trigonometric degree δ if and only if it is not also of enhanced trigonometric degree $\delta + 1$.

In view of this definition the *strict* enhanced degree can be expressed as

$$(2) \quad \delta(Q(\Lambda)) = \min_{\forall \mathbf{h} \in \Lambda^\perp; \mathbf{h} \neq \mathbf{0}} \|\mathbf{h}\|_1.$$

A *basic cell* of any lattice is the smallest nonzero volume enclosed by any s -dimensional simplex whose vertices are $s + 1$ distinct lattice points. One may show that the abscissa count of $Q(\Lambda)$, denoted by $\nu(Q)$ or $\nu(\Lambda)$, coincides with $s!V$, where V is the s -volume of the basic cell of Λ^\perp . (See, for example, [Lyn89].) Thus:

$$(3) \quad \nu(Q(\Lambda)) = s!V = |\det B| = |\det A|^{-1},$$

where B is $(A^{-1})^T$ or any other generator matrix of Λ^\perp .

Thus, two algebraic properties of the lattice rule are geometrical properties of the associated dual lattice. The enhanced degree δ is the shortest L_1 distance between any two points of the lattice, while the abscissa count is a known multiple of the volume of its basic cell.

1.3. K -optimal rules. These two geometric properties of the lattice lend plausibility to the idea that the more efficient lattice rules might have dual lattices generated by points \mathbf{h} for which $\|\mathbf{h}\|_1 = \delta$. (See [CoLy01].) The population $K(3, \delta)$ comprises integer lattices generated by three points, each located on a different pair of opposite faces of the octahedron $\|\mathbf{x}\|_1 = \delta$. The population $K(s, \delta)$ is an exact s -dimensional generalization of this. (The terms *facet-pair* and *s-crosspolytope* may be used in this context.) We refer to the optimal rules corresponding to these lattices as $K(s, \delta)$ -optimal.

This search was extremely expensive, so expensive indeed that for higher values of δ we were obliged to treat only subcategories of $K(s, \delta)$. This work is specified in detail in [CoLy01]. (A few of the abscissa counts (denoted by N_{KO}) obtained there are reproduced in Table 2 and Figure 1.) A detailed examination of the K -optimal rules obtained by this search revealed that some of them conform to a recognizable simple structure. Specifically, those listed for $\delta = 1, 2, 6, 11, 13$, and 19 (or one of their symmetric equivalents) could be generated by a skew-circulant matrix. This fact led us to define and investigate *skew-circulant lattice rules* (Sections 2 and 3).

1.4. Results for skew-circulant rules. Results of a computer search for optimal skew-circulant rules in four (and in three) dimensions are presented in Section 5 (and in Section 7). We noticed that almost all the optimal skew-circulant rules conform to a particular pattern; consequently, we were able to define for $s = 4$ and for all positive integers δ a particular skew-circulant rule denoted by $\hat{Q}(4, \delta)$. This is specified in detail in Section 5. There we show the following:

1. For *all* δ this rule is of enhanced degree δ .
2. For many values of δ including all those in the range $[23, 47]$, $\hat{Q}(4, \delta)$ is an *optimal* skew-circulant rule of enhanced degree δ .

3. There are, however, sequences of values of δ for which $\hat{Q}(4, \delta)$ is *not* an *optimal* skew-circulant rule of degree δ .

Our proof of statement 1, given in Section 5, is cumbersome, in that it requires a large but finite number of repetitive calculations. Statement 2 comprises a finite set of substatements, each of which may be verified by a moderate computer search. Statement 3 is established in Section 6 by using an argument based on the rho index of a rule.

From the point of view of matrix theory, the skew-circulant matrix is a somewhat unexciting variant of the circulant matrix. For many values of δ , however, all four-dimensional lattice rules generated by a circulant matrix require more abscissas than does the corresponding skew-circulant rule $\hat{Q}(4, \delta)$. In a search up to $\delta = 47$, only $\delta = 5$ and $\delta = 9$ appeared as exceptions.

2. SKEW-CIRCULANT MATRICES AND LATTICES

In this section, we introduce skew-circulant matrices [Dav94] and then define and discuss skew-circulant lattices.

2.1. Skew-circulant matrices. The theory in this subsection is not new. It is a straightforward modification of the corresponding theory for the classical circulant matrix. It is presented here to establish the notation.

An $s \times s$ skew-circulant matrix is one of the form

$$(4) \quad \bar{C}(\mathbf{a}) := \bar{C}(a_0, a_1, \dots, a_{s-1}) := \begin{pmatrix} a_0 & a_1 & a_2 & \dots & a_{s-1} \\ -a_{s-1} & a_0 & a_1 & \dots & a_{s-2} \\ \vdots & \vdots & \vdots & & \vdots \\ -a_2 & -a_3 & -a_4 & \dots & a_1 \\ -a_1 & -a_2 & -a_3 & \dots & a_0 \end{pmatrix}.$$

Here, and in the sequel, we use \mathbf{a} to stand for $(a_0, a_1, \dots, a_{s-1})$.

We denote by $\bar{C}^{(s)}$ the class of $s \times s$ skew-circulant matrices. Their properties are readily derived in terms of our *principal basic* skew-circulant matrix

$$(5) \quad T = \bar{C}(0, 1, 0, \dots, 0) = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ -1 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

It follows immediately that

$$(6) \quad T^i = \bar{C}(0, \dots, 0, 1, 0, \dots, 0) = \begin{pmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & 1 & \dots & 0 \\ \vdots & & & \vdots & \vdots & & \vdots \\ -1 & 0 & 0 & \dots & \dots & \cdot & 0 \\ \vdots & & & \vdots & \vdots & & \vdots \\ 0 & \dots & -1 & 0 & 0 & \dots & 0 \end{pmatrix},$$

where the unit is the $(i + 1)$ th argument of \bar{C} .

The following properties of basic skew-circulant matrices are easily established by applying the definition:³

- $\det(T) = (-1)^s$; T is unimodular.
- $T^{i+s} = -T^i$.
- $T^T T = I$; T is orthogonal.
- $(T^i)^T = -T^{s-i}$.

Note that

$$(7) \quad \bar{C}(a_0, a_1, \dots, a_{s-1}) = \sum_{i=0}^{s-1} a_i T^i$$

and that the $(j + 1)$ th row of $\bar{C}(\mathbf{a})$ is simply $\mathbf{a} T^j$, where as usual \mathbf{a} is the first row of $\bar{C}(\mathbf{a})$.

Applying these basic properties, one can easily prove a number of interesting properties for the class of skew-circulant matrices (denoted $\bar{C}^{(s)}$).

- If $A = \bar{C}(a_0, a_1, \dots, a_{s-1})$ and B are in $\bar{C}^{(s)}$, then
 - (i) $AB \in \bar{C}^{(s)}$,
 - (ii) $AB = BA$,
 - (iii) $A^T = \bar{C}(a_0, -a_{s-1}, \dots, -a_1)$,
 - (iv) $(A^{-1})^T \in \bar{C}^{(s)}$.

2.2. Skew-circulant lattices. In this paper we shall use the terminology $\Lambda(B)$ to denote the s -dimensional lattice generated by the s rows of an $s \times s$ generator matrix B .

Definition 2.1. A skew-circulant **lattice** is one that can be generated by a skew-circulant **matrix**.

This specification of a skew-circulant lattice Λ in terms of a skew-circulant generator matrix is not unique.

Theorem 2.2. *Let A be a skew-circulant matrix. Then*

$$(8) \quad \Lambda(AT^j) = \Lambda(T^j A) = \Lambda(A).$$

Proof. Since both A and T^j are skew-circulant matrices, they commute, and so the arguments in the first two members of (8) are identical. Since T^j is a unimodular matrix, Theorem 1.1 asserts that the lattices in the second and third members of (8) coincide. □

Theorem 2.2 provides $2s$ generally distinct skew-circulant matrices, namely, AT^j , $j = 0, 1, 2, \dots, 2s - 1$, each of which generates the same skew-circulant lattice.

The reader will notice that the lattice $\Lambda(\bar{C}(a_0, a_1, \dots, a_{s-1}))$ includes all the points appearing as rows of $\bar{C}(a_0, a_1, \dots, a_{s-1})$ together with their negatives. Thus this lattice includes the set of $2s$ points $\mathbf{a} T^j$, $j = 0, 1, \dots, 2s - 1$. This is a special case of the following.

Definition 2.3. A set of $2s$ points of the form $\mathbf{x} T^j$, $j = 0, 1, \dots, 2s - 1$, is termed a *skew-circulant set of points* related to \mathbf{x} .

³A superscript T denotes the matrix transpose. Here, $(T^i)^T$ denotes the transpose of the matrix T^i .

Theorem 2.4. *When \mathbf{x} is any element of a skew-circulant lattice Λ , all skew-circulant points related to \mathbf{x} are also elements of Λ .*

Proof. $\mathbf{x} \in \Lambda(A)$ implies that there exists a λ such that $\mathbf{x} = \lambda A$. It follows that $\mathbf{x}T^j = \lambda AT^j$, which is the condition that $\mathbf{x}T^j \in \Lambda(AT^j)$. In view of Theorem 2.2 $\Lambda(AT^j) = \Lambda(A)$, which establishes Theorem 2.4. \square

The dual Λ^\perp of any lattice $\Lambda(B)$ is the lattice generated by $(B^{-1})^T$. In view of the last result of the preceding section, Λ^\perp is a skew-circulant lattice whenever Λ is.

The reader should bear in mind that a matrix that is not skew-circulant may, on occasion, generate a skew-circulant lattice. Let B be any integer matrix and let $\Lambda(B)$ be the lattice it generates. It follows that $\Lambda(B)$ is a skew-circulant lattice if and only if there exists a unimodular matrix U such that UB may be expanded in the form

$$(9) \quad UB = \sum_{i=0}^{s-1} a_i T^i.$$

3. LATTICES AND THEIR EQUIVALENCE CLASSES

In constructing a search over any population, there is usually a major cost reduction if the natural symmetry of the population can be exploited in some way. A *symmetric copy* of a lattice is another lattice obtained from the first by any sequence of those affine transformations that take the unit lattice into itself.

Lattices that are symmetric copies of each other are said to belong to the same *equivalence class*. They share many of the same characteristics. In the present context the most important features appear to be that they obviously share the same trigonometric degree and order. Thus, in any search for optimal skew-circulant lattice rules there is no need in principle to consider more than one member of each equivalence class.

In terms of generator matrices, symmetric copies of a lattice may be created by postmultiplying by permutation matrices and sign change matrices.

In the rest of this section, the theorems will be stated in an s -dimensional context. However, much of the discussion will be presented in a four-dimensional context.

Let \mathcal{G}_i be an element of the group \mathcal{G} of 384 affine transformations that takes the hypercube $[0, 1]^4$ into itself. Let G_i be a standard⁴ matrix representation of \mathcal{G}_i . (We abbreviate this to $G_i \in \mathcal{G}$.) Let A be a generator matrix of a lattice $\Lambda(A)$. Then the set of lattices in the equivalence class that contains A comprises all lattices $\Lambda(AG_i)$, $i = 1, 2, \dots, 384$. These lattices are not distinct; when $G_i = -G_k$, the lattices $\Lambda(AG_i)$ and $\Lambda(AG_k)$ coincide. However, 192 elements of this set may be distinct. On the other hand, the class may have many fewer elements. In the extreme case, when $\Lambda(A)$ is a multiple of the unit lattice, then all members of this set coincide, and the equivalence class contains only one member.

Definition 3.1. $\Lambda(A)$ and $\Lambda(\tilde{A})$ are members of the same equivalence class, written

$$\Lambda(A) \equiv \Lambda(\tilde{A}),$$

if and only if there exists a unimodular matrix U and a permutation matrix $G \in \mathcal{G}$ such that $\tilde{A} = UAG$.

⁴ For any matrix A , the matrix AG_i may be constructed by applying \mathcal{G}_i to the *columns* of A .

We note that the elements T^j , $j = 0, 1, \dots, 7$, introduced in (5) and (6) are themselves matrix representations G_k of elements of the group \mathcal{G} . These elements form a subgroup of order 8. We introduce the set of 48 right cosets of this subgroup; these are

$$(10) \quad \{T^j G_k : j = 0, 1, \dots, 7; \}, \quad k = 1, 2, \dots, 48.$$

It is known from elementary group theory that G_k , $k = 1, 2, \dots, 48$, may be chosen in such a way that these cosets are disjoint and the union of their members comprise the totality of the members of \mathcal{G} .

Theorem 3.2. *When an s -dimensional equivalence class contains a skew-circulant lattice $\tilde{\Lambda}$, the class can contain no more than $2^{s-1}(s-1)!$ distinct lattices.*

Proof. Let A be a skew-circulant matrix that generates the skew-circulant lattice $\tilde{\Lambda}$ and $G \in \mathcal{G}$. Since both A and T^j are skew-circulant matrices, they commute; it follows that

$$(11) \quad \Lambda(AT^j G) = \Lambda(T^j AG) = \Lambda(AG), \quad j = 0, 1, \dots, 7.$$

Thus, when G' and G'' are members of the same coset specified in (10), the lattices $\Lambda(AG')$ and $\Lambda(AG'')$ coincide. Since there are at most only 48 distinct cosets, there are at most only 48 distinct lattices in this equivalence class. \square

By hypothesis one of these is a skew-circulant lattice. The following theorems show that, when s is *even*, there are three more in general. In four dimensions, we have not encountered any equivalence class having more than four distinct skew-circulant lattices. (No theorem to this effect is known to us.)

The next two theorems depend on a suitable choice of a unimodular matrix U and of $G \in \mathcal{G}$ for use in the relation

$$(12) \quad \Lambda(UAG) \equiv \Lambda(A).$$

Theorem 3.3. *Let $A = \bar{C}(a_0, a_1, \dots, a_{s-1})$ and $\tilde{A} = \bar{C}(a_{s-1}, a_{s-2}, \dots, a_0)$. Then $\Lambda(A) \equiv \Lambda(\tilde{A})$.*

Proof. Define

$$(13) \quad P = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 1 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}.$$

It is readily confirmed that $PT^jP = -T^{s-j}$; since $A = \sum_{j=0}^{s-1} a_j T^j$, it follows that

$$(14) \quad -T^{-1}PAP = -T^{-1} \sum_{j=0}^{s-1} a_j PT^jP = T^{-1} \sum_{j=0}^{s-1} a_j T^{s-j} = \bar{C}(a_{s-1}, a_{s-2}, \dots, a_0).$$

Setting $U = -T^{-1}P$ and $G = P$ in (12) establishes the theorem. \square

Theorem 3.4. For even s , $\Lambda(A) \equiv \Lambda(A_-)$, where $A = \bar{C}(a_0, a_1, \dots, a_{s-1})$ and $A_- = \bar{C}(a_0, -a_1, a_2, -a_3, \dots, -a_{s-1})$.

Proof. Let

$$(15) \quad S = \text{diag}(1, -1, 1, -1, \dots, 1, -1).$$

It is readily verified that $SAS = A_-$. Setting $U = G = S$ in (12) establishes the theorem. \square

4. A SEARCH

Many extensive searches for optimal lattice rules are described in the literature. Beside these, our simple search for efficient skew-circulant lattice rules in three and four dimensions appears to be almost trivial. This is because the population $\bar{C}^{(s)}$ of skew-circulant lattices is relatively small.⁵

Definition 4.1. The lattice Λ is a $\bar{C}^{(s)}$ -optimal lattice of (strict) enhanced degree δ when any other $\bar{C}^{(s)}$ lattice Λ' of (strict) enhanced degree δ satisfies $\nu(\Lambda') \geq \nu(\Lambda)$.

To find a $\bar{C}^{(s)}$ -optimal lattice of strict enhanced degree $\tilde{\delta}$, it is sufficient to test every integer lattice $\Lambda(B)$ generated by $B = \bar{C}(b_0, b_1, \dots, b_{s-1})$ having

$$(16) \quad |b_0| + |b_1| + |b_2| + \dots + |b_{s-1}| = \tilde{\delta}.$$

Since simple analytical formulas for $\det B$ exist, the abscissa count

$$(17) \quad \nu(B) = |\det B|$$

is significantly easier to calculate than the enhanced degree $\delta(B)$. We calculate $\nu(B)$ for each lattice of this set. We retain the first lattice encountered for which $\delta(B) = \tilde{\delta}$ as the first entry on our provisional list of optimal candidates. Subsequently, only when a new abscissa count $\nu(B)$ is found to be less than or equal to the current provisional count is it necessary to calculate $\delta(B)$. If this coincides with our target enhanced degree $\tilde{\delta}$, we retain this lattice on our provisional list. If the new abscissa count is less than the current provisional count, all other members of this list are discarded. At the completion of such a search, a complete list of $\bar{C}^{(s)}$ -optimal lattices remains.

Short though this search appears to be, it turns out that in four dimensions the population (16) can be curtailed. One needs to include only those $\Lambda(B)$ for which all components of \mathbf{b} are nonnegative (that is, \mathbf{b} is in the principal four-dimensional quadrant). Moreover, in view of Theorem 3.2, we may further restrict the search to omit \mathbf{b} when $b_3 < b_0$ and also when both $b_3 = b_0$ and $b_2 < b_1$. In view of Theorem 2.2, the skew-circulant lattice generated by $\mathbf{b}T^j$ coincides with the lattice generated by \mathbf{b} . And, according to Theorem 3.4, the lattice generated by $\mathbf{b}S$ is symmetrically equivalent to the one generated by \mathbf{b} . (S is defined in (15) above.) Merely by checking these sign patterns, one can verify that in four dimensions the sixteen points $\mathbf{b}T^j$ and $\mathbf{b}T^jS$ lie, respectively, in each of the sixteen distinct octants.

The corresponding situation in more than four dimensions is more complicated and is not discussed here. Even in three dimensions a different situation prevails. For example, the rule generated by $\bar{C}(1, -3, 6)$ is an optimal skew-symmetric rule of degree $\delta = 10$. But the set of rules which may be generated by $\bar{C}(\mathbf{b})$ with all

⁵ Depending on the context, $\bar{C}^{(s)}$ may refer to the set of skew-circulant matrices, the set of skew-circulant lattices, or the set of skew-circulant lattice rules.

components of \mathbf{b} nonnegative does not include this rule, nor does it include any optimal skew-symmetric rule with $\delta = 10$.

5. THE SEQUENCE OF LATTICE RULES $\hat{Q}(4, \delta)$

In dimension $s = 4$ for all $\delta \leq 47$ we have carried out a search for all the optimal four-dimensional skew-circulant rules of enhanced degree δ .

As mentioned in Section 1, detailed examination of these results indicates that, for all $\delta \in [23, 47]$ the lattice rule $\hat{Q}(4, \delta)$ specified below is an optimal skew-circulant rule of strict enhanced degree δ , and all other optimal skew-circulant rules of the same strict degree are in the same equivalence class as this one. \hat{Q} may be specified as follows.

Definition 5.1. Let $\delta = 6k + r$, where $r \in [0, 5]$. Define $\hat{\mathbf{b}}(4, \delta)$ as indicated in Table 1. Then \hat{Q} is the lattice rule $Q(\hat{\Lambda})$, where $\hat{\Lambda}$ is the dual of the lattice $\hat{\Lambda}^\perp$ generated by $\hat{B} = \bar{C}(\hat{\mathbf{b}})$.

In the lower half of Table 1 we provide the components of a skew-circulant integer matrix

$$\tilde{A} = \bar{C}(\tilde{a}_0, \tilde{a}_1, \tilde{a}_2, \tilde{a}_3),$$

which is a scaled version of \hat{A} , a generator matrix of $\hat{\Lambda}$. These elements are all cubic polynomials in k . Specifically,

$$\hat{A} = (\hat{B}^T)^{-1} = \tilde{A}/\hat{N}.$$

Besides being an optimal skew-circulant rule for all $\delta \in [23, 47]$, the rule $\hat{Q}(4, \delta)$ is also an optimal skew-circulant rule for all values of $\delta \in [1, 22]$ with the following five exceptions. For $\delta = 4, 10, 16, 22$ the rules generated by $\bar{C}(\mathbf{b})$ with $\mathbf{b}(4, 6k + 4) = (0, 3k + 2, 2k + 1, k + 1)$, and for $\delta = 3$, the rule generated by $\bar{C}(1, 0, 1, 1)$ are $\bar{C}^{(s)}$ -optimal.

TABLE 1. Parameters for specification of $\hat{Q}(4, \delta)$ for positive integer δ .

r	$\hat{\mathbf{b}}(4, 6k + r)$	δ	\hat{N}
0	$(0, 3k, 2k, k)$	$6k$	$68k^4$
1	$(1, 3k + 1, 2k, k - 1)$	$6k + 1$	$68k^4 + 48k^3 + 28k^2 + 8k + 1$
2	$(0, 3k + 1, 2k + 1, k)$	$6k + 2$	$68k^4 + 88k^3 + 52k^2 + 16k + 2$
3	$(1, 3k + 2, 2k + 1, k - 1)$	$6k + 3$	$68k^4 + 136k^3 + 136k^2 + 68k + 17$
4	$(0, 3k + 2, 2k + 2, k)$	$6k + 4$	$68k^4 + 176k^3 + 208k^2 + 128k + 32$
5	$(1, 3k + 3, 2k + 1, k)$	$6k + 5$	$68k^4 + 232k^3 + 312k^2 + 196k + 49$

r	$-\tilde{a}_0$	\tilde{a}_1	$-\tilde{a}_2$	$-\tilde{a}_3$
0	$16k^3$	$26k^3$	$4k^3$	$2k^3$
1	$16k^3 + 6k^2 + 4k + 1$	$26k^3 + 14k^2 + 7k + 1$	$4k^3 + 2k$	$2k^3 + 6k^2 + 3k + 1$
2	$16k^3 + 20k^2 + 8k + 1$	$26k^3 + 24k^2 + 8k + 1$	$4k^3 - 2k^2 - 4k - 1$	$2k^3 + 10k^2 + 6k + 1$
3	$16k^3 + 26k^2 + 18k + 5$	$26k^3 + 38k^2 + 25k + 6$	$4k^3 - 2k^2 - 4k - 3$	$2k^3 + 16k^2 + 15k + 7$
4	$16k^3 + 40k^2 + 32k + 8$	$26k^3 + 48k^2 + 32k + 8$	$4k^3 - 4k^2 - 16k - 8$	$2k^3 + 20k^2 + 24k + 8$
5	$16k^3 + 34k^2 + 26k + 7$	$26k^3 + 68k^2 + 63k + 21$	$4k^3 + 14k^2 + 16k + 7$	$2k^3 + 2k^2 + k$

For several randomly chosen values of $\delta \in [48, 120]$ the same search was carried out. No counterexample to the (incorrect) conjecture that $\hat{Q}(4, \delta)$ is optimal for all $\delta \geq 23$ was discovered in this way. Later, however, we show theoretically (see Theorem 6.2) that such a conjecture is false.

The rest of this section is devoted to establishing Theorem 5.3; in the proof we shall employ the following well-known inequality.

Lemma 5.2. *Let A be the generator matrix of an integration lattice Λ , and let $B = (A^T)^{-1}$. Let $\mathbf{h} = \lambda B$ with $\lambda \in \Lambda_0$. Then*

$$\|\mathbf{h}\|_1 \geq \|\lambda\|_1 / \|A\|_1.$$

Proof. It follows immediately from the hypothesis that $A\mathbf{h}^T = \lambda^T$. Applying a standard L_1 inequality to this yields the result. \square

Theorem 5.3. *For all $k \geq 0$ and $r = 0, 1, \dots, 5$, the four-dimensional skew-circulant rule $\hat{Q}(4, 6k + r)$ specified in Table 1 has enhanced degree $\delta = 6k + r$.*

This can be verified numerically for any individual value of k . So we do not compromise the proof when, at one point, we restrict k to exceed 2. There is no need to treat $r = 0$ because $\hat{Q}(4, 6k)$ is the k -copy version of $\hat{Q}(4, 6)$, and so the theorem is self-evident. And since $\hat{Q}(4, 12k + 4)$ is the 2-copy version of $\hat{Q}(4, 6k + 2)$, the case $r = 2$ need not be treated so long as the case $r = 4$ is treated. However, we do not exploit this, and the proof below applies to all r .

Proof. We shall establish the theorem by showing that each nonzero element \mathbf{h} of each dual lattice $\hat{\Lambda}^\perp$ satisfies $\|\mathbf{h}\|_1 \geq \delta$.

The proof falls into two parts. In Lemma 5.4, we apply Lemma 5.2 to show that when $\|\lambda\|_1 \geq 5$, the corresponding \mathbf{h} has 1-norm larger than or equal to $6k + r$. In Lemma 5.5, we simply record the result of computing $\|\mathbf{h}\|_1$ for the remaining elements of $\hat{\Lambda}^\perp$. For each δ there are 240 of these, corresponding to $\|\lambda\|_1 \leq 4$.

Theorem 5.3 is an immediate consequence of these two lemmas. \square

Lemma 5.4. *For all $k \geq 0$ and $r = 0, 1, \dots, 5$, with \hat{A} and $\delta = 6k + r$ as specified in Table 1, when both $\lambda \in \Lambda_0$ and $\|\lambda\|_1 \geq 5$, it appears that $\|\lambda\|_1 / \|A\|_1 \geq \delta$.*

Proof. The elements of the skew-circulant matrix \tilde{A} are given in the lower part of Table 1 and the elements of \hat{A} are \tilde{A}/\hat{N} . The right-hand side of the inequality in Lemma 5.2 is

$$(18) \quad \|\lambda\|_1 \hat{N}/\hat{D},$$

where

$$(19) \quad \hat{D} = -\tilde{a}_0 + \tilde{a}_1 - \tilde{a}_2 - \tilde{a}_3$$

for all $k > 2$.

For fixed r , \hat{N} is a quartic and \hat{D} a cubic polynomial in k . All the coefficients of these polynomials are nonnegative. Carrying out the calculation for each $r = 0, 1, \dots, 5$ in turn, we find that the coefficient of each power of k in $(6k + r)\hat{D}(r)$ is less than the corresponding coefficient in $5\hat{N}(r)$, and consequently,

$$(20) \quad (6k + r)\hat{D}(r) < 5\hat{N}(r).$$

It follows that, when $\|\lambda\|_1 \geq 5$,

$$(21) \quad \|\lambda\|_1 \hat{N}/\hat{D} \geq 5\hat{N}/\hat{D} > 6k + r,$$

as required by the lemma. □

Lemma 5.5. *For all $k \geq 0$ and $r = 0, 1, \dots, 5$, with \hat{B} and $\delta = 6k + r$ as specified in Table 1, for $\lambda \in \Lambda_0$ and $\|\lambda\|_1 \leq 4$ the elements of $\mathbf{h} = \lambda \hat{B}$ satisfy $\|\mathbf{h}\|_1 \geq \delta$.*

Proof. We treat separately each value of r . For a fixed value of r , and for one of the 240 instances corresponding to $\|\lambda\|_1 \leq 4$, we calculate $\mathbf{h}^T = \lambda^T \hat{B}$ and form $\|\mathbf{h}\|_1$. Since \hat{B} is the skew-circulant matrix specified in Table 1, we find

$$\begin{aligned} \|\mathbf{h}\|_1 &= |\lambda_1 \hat{b}_0 + \lambda_2 \hat{b}_1 + \lambda_3 \hat{b}_2 + \lambda_4 \hat{b}_3| \\ &\quad + |-\lambda_1 \hat{b}_3 + \lambda_2 \hat{b}_0 + \lambda_3 \hat{b}_1 + \lambda_4 \hat{b}_2| \\ &\quad + |-\lambda_1 \hat{b}_2 - \lambda_2 \hat{b}_3 + \lambda_3 \hat{b}_0 + \lambda_4 \hat{b}_1| \\ &\quad + |-\lambda_1 \hat{b}_1 - \lambda_2 \hat{b}_2 - \lambda_3 \hat{b}_1 + \lambda_4 \hat{b}_0|. \end{aligned}$$

Here each element \hat{b}_i is the linear function of k appearing in the r th line of the upper part of Table 1. We have to show that this expression of $\|\mathbf{h}\|_1$, in terms of k , is not less than $\delta = 6k + r$.

In fact, we verified very few of these computations by hand. A computer program was then constructed to carry out this calculation for all 240 assignments of λ and all six assignments of r . □

6. ABSCISSA COUNTS

We now briefly discuss the relative efficiency of these skew-circulant rules when compared with existing rules.

In Table 2 we have listed various abscissa counts for $\delta \leq 30$. These are as follows:

- N_{ME} , a theoretical lower bound on the number of abscissas required by any rule of this degree [CoSl96],
- N_{KO} , the lowest abscissa count of any K -optimal rule listed in [CoLy01],
- $N_{\bar{CO}}$, the abscissa count for the optimal skew-circulant rule,
- \hat{N} , the abscissa count for $\hat{Q}(4, \delta)$, calculated from the expression in Table 1.

The reader will notice that, on any particular line in the table, the entries are in nondecreasing order. This follows principally because the corresponding rules are optimal with respect to successively smaller populations.

Examination of this table shows that the optimal skew-circulant rule is also a K -optimal rule in the cases $\delta = 2, 6, 11, 13$, and 19. For some other *odd* values of δ , $N_{\bar{CO}}$ is very close to N_{KO} . But for *even* values of δ , this difference is larger, up to four percent.

To obtain a visual impression of the relative efficiency of these rules, we have used the recently introduced rho index $\rho(Q)$, which is defined as follows.

Definition 6.1. The *rho index* $\rho(Q)$ of any s -dimensional cubature rule Q for $[0, 1]^s$ of *strict* enhanced degree δ and abscissa count N is

$$(22) \quad \rho(Q) = \frac{\delta^s}{N \cdot s!}.$$

This index was introduced in [CoLy01] and has been discussed at some length in [LyCo00]. It appears that the value of this index for any m -copy of Q is the same as its value for Q . And the value of the index cannot exceed 1.

TABLE 2. Four-dimensional abscissa counts. (The value of $N_{\bar{C}O}$ is not shown for values of δ for which $N_{\bar{C}O} = \hat{N}$.)

δ	N_{ME}	N_{KO}	$N_{\bar{C}O}$	\hat{N}
1	1	1		1
2	2	2		2
3	9	9	9	17
4	16	16	18	32
5	41	45		49
6	66	68		68
7	129	152		153
8	192	212		226
9	321	375		425
10	450	516	562	612
11	681	857		857
12	912	1064		1088
13	1289	1601		1601
14	1666	1958		2034
15	2241	2834		2873
16	2816	3312	3554	3616
17	3649	4628		4633
18	4482	5354		5508
19	5641	7081		7081
20	6800	8148		8402
21	8361	10552		10625
22	9922	11886	12546	12548
23	11969	15167		15217
24	14016	16812		17408
25	16641			20961
26	19266			23938
27	22569			28577
28	25872			32544
29	29961			38081
30	34050			42500

A plot of rho indices of various optimal rules having $\delta \leq 30$ appears in Figure 1. The information required for each entry in this figure appears in Table 2. Naturally, in Figure 1 and Table 2 are simply different ways of presenting the identical information.

We may exploit some of this information to demonstrate the falsity of the conjecture that, for sufficiently high δ , the rule $\hat{Q}(4, \delta)$ might always be an optimal skew-circulant rule.

Theorem 6.2. *When δ is of the form $18k + 6$ with $k \geq 4$ or when δ is of the form $18k + 12$ with $k \geq 7$, the skew-circulant rule $\hat{Q}(4, \delta)$ is not an optimal skew-circulant rule.*

Proof. The three-copy version of $\hat{Q}(4, 6k + 2)$ is a skew-circulant rule of degree $18k + 6$. When $k \geq 4$, its rho index $\hat{\rho}(6k + 2)$ exceeds the rho index $\hat{\rho}_{\text{lim}}$ of $\hat{Q}(4, 18k + 6)$. Thus $\hat{Q}(4, 18k + 6)$ is not optimal. The other result in the theorem is proved in the same way. \square

7. THREE-DIMENSIONAL THEORY AND RESULTS

In the preceding two sections we have described at some length some of our results in our search for optimal four-dimensional skew-circulant lattice rules. We have also carried out a corresponding search in three dimensions for optimal rules of strict enhanced degree δ up to enhanced degree $\delta = 60$. The results are less interesting. We outline some of them here.

As in the four-dimensional case, the search provided a sequence of optimal skew-circulant rules. We have identified an infinite sequence of skew-circulant rules $\hat{Q}(3, \delta)$, which are specified in Table 3. For all $\delta \leq 60$, with eleven exceptions (namely, $\delta = 5, 7, 8, 10, 11, 13, 14, 17, 20, 26$, and 32), it appears that $\hat{Q}(3, \delta)$ is an optimal skew-circulant rule of *strict* enhanced degree δ .

In three dimensions, as in all dimensions, optimal rules are known for enhanced degrees $\delta = 1, 2, 3, 4$. In three dimensions only, an optimal rule is also known for $\delta = 6$. This is based on Minkowski’s celebrated *critical* lattice, stemming from classical lattice theory [Min11], which provides a lattice and lattice rule of enhanced degree $\delta = 6$. In our context, this theory also provides an upper bound $\rho_{CL} = 18/19$ on the rho index of any three-dimensional *lattice* rule. Since all m -copies $\hat{Q}(3, 6m)$ of this rule share the same rho index, these copies are all optimal *lattice* rules.

In [CoLy01] a list of three-dimensional K -optimal lattices appears for $\delta \in [1, 30]$. For $\delta = 6k$ these are the optimal lattice rules $\hat{Q}(3, 6)$ just mentioned. For $\delta = 6k + 3 \leq 30$, these coincide with one of the optimal skew-circulant rules $\hat{Q}(3, 6k + 3)$. For $\delta = 6k + r \leq 30$ with $r = 1, 2, 4, 5$, however, the optimal skew-circulant rules are inferior to known K -optimal rules.

TABLE 3. Parameters for specification of $\hat{Q}(3, \delta)$ for positive integer δ .

r	$\hat{\mathbf{b}}(3, 6k + r)$			$\frac{\hat{N}}{\ \hat{\mathbf{a}}\ _1}$	$\ \hat{\mathbf{a}}\ _1$	$\hat{\mathbf{a}}(3, 6k + r)$		
0	k	$2k$	$3k$	$2k$	$19k^2$	$7k^2$	$-k^2$	$11k^2$
1	k	$2k$	$3k+1$	$2k+1$	$19k^2+7k+1$	$7k^2+2k$	$-(k-1)k$	$11k^2+6k+1$
2	$k+1$	$2k$	$3k+1$	$2k+1$	$19k^2+8k+1$	$7k^2+4k+1$	$-(k^2-4k-1)$	$11k^2+8k+1$
3	k	$2k+1$	$3k+2$	$2k+1$	$19k^2+22k+7$	$7k^2+7k+2$	$-(k+1)^2$	$11k^2+13k+4$
4	$k+1$	$2k+1$	$3k+2$	$2k+2$	$19k^2+23k+7$	$7k^2+9k+3$	$-(k^2-k-1)$	$11k^2+15k+5$
5	$k+1$	$2k+1$	$3k+3$	$2k+3$	$19k^2+30k+12$	$7k^2+11k+4$	$-(k^2-2k-2)$	$11k^2+21k+10$

One disconcerting feature of these results is that, for $k \geq 2$, our rule $\hat{Q}(3, 6k + 5)$ actually uses more function values than does $\hat{Q}(3, 6k + 6)$. This is possible because definitions and searches are restricted to rules of *strict* enhanced degree δ ; that is, they exclude any of degree exceeding δ .

Definition 7.1. Let $\delta = 6k + r$, where $r \in [0, 5]$. Define $\hat{\mathbf{b}}(3, \delta)$ as indicated in Table 3. Then \hat{Q} is the lattice rule $Q(\hat{\Lambda})$, where $\hat{\Lambda}$ is the dual of the lattice $\hat{\Lambda}^\perp$ generated by $\hat{B} = \bar{C}(\hat{\mathbf{b}})$.

The table includes a specification of other quantities required to construct the rule directly. These are defined in the proof of the following theorem.

Theorem 7.2. Let a, b, c be nonnegative integers such that $b^2 \geq ac$. Let $B = \bar{C}(a, b, c)$ and $A = (B^{-1})^T$. Then $\|A\|_1 = 1/(a - b + c)$.

Proof. One finds by simple manipulation that

$$(23) \quad \det B = a^3 - b^3 + c^3 + 3abc = (a - b + c)(a^2 + b^2 + c^2 + ab + bc - ca).$$

It is simple to verify that $A = (B^{-1})^T = \bar{C}(\tilde{\mathbf{a}})/\det B$ with

$$(24) \quad \tilde{\mathbf{a}} = (a^2 + bc, -(c^2 + ab), b^2 - ca).$$

Up to this point a, b , and c can be general. When a, b , and c are nonnegative and $b^2 > ac$, we find

$$(25) \quad \|A\|_1 = (a^2 + b^2 + c^2 + ab + bc - ca)/\det B,$$

and in view of (23) we find $\|A\|_1 = 1/(a - b + c)$. □

In Table 3, we list, for each $\delta = 6k + r$, the quantities $\hat{\mathbf{b}}, \hat{N}, \|\tilde{\mathbf{a}}\|_1$, and $\tilde{\mathbf{a}}$ as functions of k . These may be obtained from the corresponding quantities in the proof of the theorem by replacing (a, b, c) by $\hat{\mathbf{b}}$.

With the exception of enhanced degrees $\delta = 5, 7, 8, 11, 13$, and 17 these are optimal skew-circulant rules of *strict* degree δ for $\delta \in [1, 60]$. We have no proof that these are optimal for all $\delta > 61$. And we have no counterexamples to refute such a conjecture. As mentioned above, however, we have established that $\hat{Q}(3, \delta)$ is of enhanced degree δ for all δ .

Theorem 7.3. For all $k \geq 0$ and $r = 0, 1, \dots, 5$, the three-dimensional skew-circulant rule $\hat{Q}(3, 6k + r)$ specified in Table 3 has enhanced degree $\delta = 6k + r$.

The proof is along the same lines as the proof of Theorem 5.3 but is much simpler. It appears that in the three-dimensional version of Lemma 5.4 we need to restrict λ to $\|\lambda\|_1 \geq 3$. The number of simple computations to establish the three-dimensional version of Lemma 5.5 becomes far fewer, in part because of the reduced dimension and in part because of the lower limit on $\|\lambda\|_1$.

8. CONCLUDING REMARKS

The results in this paper contribute to the theory of multidimensional numerical quadrature rules for $[0, 1]^s$ having specified *trigonometric* degree. For $s \geq 4$, optimal rules are known only for $\delta \leq 4$. All available rules of higher degree are copies of these or have been discovered empirically, nearly always by means of intensive computer-based searches. A reduction of the population that is searched produces rules optimal only within the smaller population but at a lower cost. Thus, while we

would prefer to find optimal rules, we have used computer searches to find optimal *lattice* rules, K -optimal rules, and, as described in this paper, optimal *skew-circulant* rules. Each population considered is a subset of the previous population. Each of the final three requires only a finite search. Naturally, each search is shorter than the corresponding previous one and yields less efficient results.

The search over skew-circulant rules (described in Section 4) is intrinsically much shorter than the more thoroughgoing searches mentioned above. It may be much more efficient, however, because of the underlying situation with respect to duplicate copies and symmetric copies. In the absence of special measures, a search might examine the same rule (specified by different generator matrices) several times. Moreover, the search might treat many members of the same equivalence class. Such a class may contain up to 192 distinct rules, all geometrically equivalent. The success or failure of a long search depends critically on the extent to which the search is capable of avoiding duplicate copies and symmetric copies of rules that have already been examined. In this respect, the remarks at the end of Section 4 indicate that our four-dimensional search treats each rule only once. And, by limited inspection, we have noticed that in general the four-dimensional search treats only two distinct members of each equivalence class.

In the corresponding search for K -optimal rules, it is possible that the identical rule be treated up to eight or sixteen times, and all 192 symmetric copies might also be treated with the same abandon. In practice, empirical evidence suggests an overall redundancy exceeding ninety-nine percent. (See Section 5 of [CoLy01].)

In an *odd*-dimensional context, one may show that every skew-circulant rule has a symmetrically equivalent circulant rule and vice versa. (This may be established by using a trivial variant of Theorem 3.3.) Hence an optimal *odd*-dimensional skew-circulant rule has the same abscissa count as a corresponding optimal circulant rule.

But in four (and in other *even*) dimensions the equivalence set of a circulant rule may or may not contain skew-circulant rules. Examination of four-dimensional results in the present paper and in [CoLy01] reveals the following situation. For $\delta = 1, 5$, and 9 , the optimal circulant rule coincides with a K -optimal rule and is more economic than any skew-circulant rule of the same degree. For $\delta = 1, 2, 6, 11, 13$ and 19 , the optimal skew-circulant rule coincides with a K -optimal rule. For all $\delta \in [2, 47]$, with the exceptions of 5 and 9 , the optimal skew-circulant rule is more economic than the corresponding optimal circulant rule.

Besides describing a somewhat complex situation with respect to optimal rules for large and for small values of δ , the main result of this work (illustrated in Figure 1) may be the specification of an infinite sequence of rules, one for each value of δ . For $\delta > 10$ all of these have rho indices between 0.70 and 0.80 , the limit exceeding 0.79 . (The highest four-dimensional rho index known to us at this time is 0.825 .) While some of these rules may be useful in practice, we feel that the main contribution of this paper is theoretical, establishing the existence of such a sequence.

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