The Structure and Average Discrepancies of Lattice Rules for Numerical Integration

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Abstract

Lattice rules are equal-weight quadrature rules which are used in the approximation of multidimensional integrands over the s-dimensional unit cube $[0,1]^s$. One of the problems encountered in the study of such rules is the unavailability of a unique representation. It is known that any lattice rule may be expressed in a canonical $D - Z$ form in which D is a diagonal matrix whose diagonal entries are known as the invariants and Z is an integer matrix. Although D is unique in this canonical form, Z may be chosen in many different ways. Except for the case of so-called projection-regular and prime-power rules, no such unique Z is available. In the latter case of prime-power rules, the unique $D - Z$ form developed is known as an ultratriangular form. Associated with each ultratriangular form is a set of column indices. Any lattice rule may be decomposed into prime-power components. In this thesis, a unique $D - Z$ form is defined for a special class of lattice rules for which the component prime-power rules have a consistent set of column indices. This new unique form includes the known unique forms for projection-regular and prime-power rules as special cases. We also use the ultratriangular form for prime-power lattice rules to derive a formula to calculate the number of prime-power rules having a given set of invariants and column indices.

The existing theory of lattice rules that is based on the generator matrix of the dual lattice has made the assumption that its representation in the so-called Hermite normal form is upper triangular. However, since projection-regular rules have a unique Z-matrix which is unit upper triangular, the corresponding generator matrix for the dual lattice is lower triangular. This suggests that a lower triangular Hermite normal form might be appropriate for study. We consider this situation and give the conditions on the lower triangular Hermite normal form which allow a projection-regular rule to be easily recognized.

Number-theoretic rules are a class of lattice rules which are known to be particularly suitable for the approximation of multidimensional integrals in which the integrands are periodic. In the case of non-periodic integrands there is numerical evidence that the average L_2 discrepancy for these rules is smaller than the expected value for Monte-Carlo rules when the dimension s is less than 18. For non-periodic integrands, a vertex-modified version of the number-theoretic rule has been previously proposed. In s-dimensions these vertex-modified rules contain 2^s weights

which may be chosen optimally so that the discrepancy is minimized. We shall compare the average discrepancy for these optimal vertex-modified number-theoretic rules with that for normal number-theoretic and Monte-Carlo rules. A similar comparison is also carried out between the averages for number-theoretic rules and for 2^s copy rules with approximately the same number of points.

In the case of periodic integrands it has been shown that the average of P_α and the values of R for 2^s copy rules are smaller than those for number-theoretic rules. For this periodic case, we use an analogue of the L_2 discrepancy to carry out a similar comparison.

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Contents

Chapter 1

Introduction

1.1 Numerical multiple integration

For the numerical evaluation of an s-dimensional integral over the unit cube,

$$I(f) = \int_{[0,1]^s} f(\mathbf{t})\,\mathrm{d}\mathbf{t}, \tag{1.1}$$

various methods have been proposed. Amongst these methods, commonly-used ones are Monte Carlo and quasi-Monte Carlo methods. They are equal-weight quadrature rules of the form

$$Q(f) = \frac{1}{n}\sum_{i=0}^{n-1} f(\mathbf{t}_i), \tag{1.2}$$

where the quadrature points $\mathbf{t}_0, \ldots, \mathbf{t}_{n-1}$ are appropriately chosen. When the points are randomly chosen from $[0,1]^s$; that is, the points are independent and uniformly distributed on $[0,1]^s$, rule (1.2) is known as a Monte Carlo rule. It is known as a quasi-Monte Carlo rule when the points are chosen in some deterministic manner. In this thesis, we shall be particularly concerned with a special class of quasi-Monte Carlo rules which are known in the literature as lattice rules.

Lattice rules get their name from the word "lattice". An s-dimensional lattice is a discrete set of points in $\mathbb{R}^s$ which is closed under normal addition and subtraction. It is a multiple integration lattice Λ if it contains as a subset the unit lattice,

$$\{(\ell_1, \ell_2, \ldots, \ell_s) : \ell_j \in \mathbb{Z}, \quad j = 1, 2, \ldots, s\}.$$

Here, $\mathbb{Z}$ denotes the set of integers. A lattice rule is any rule of the form

$$Q_\Lambda(f) = \frac{1}{n}\sum_{i=0}^{n-1} f(\mathbf{t}_i), \tag{1.3}$$

where the quadrature points $\mathbf{t}_0, \ldots, \mathbf{t}_{n-1}$ belong to the set $\mathcal{A}(Q)$ defined by

$$\mathcal{A}(Q) = \Lambda \cap [0,1)^s.$$

The number of distinct quadrature points in a lattice rule Q_Λ is known as the order of the rule and is denoted by $\nu(Q_\Lambda)$. If the order of a lattice rule is a prime-power; that is, $\nu(Q_\Lambda) = p^\beta$, for some prime p and positive integer β, then the lattice rule is known as a prime-power rule.

In one dimension, the only lattice rule of order n is the rectangle rule

$$R(f) = \frac{1}{n}\sum_{i=0}^{n-1} f\left(\frac{i}{n}\right). \tag{1.4}$$

Thus lattice rules may be considered to be multidimensional generalizations of this rectangle rule. If the integrand f is periodic, then in the one-dimensional case the rectangle rule is equivalent to the trapezoidal rule

$$T(f) = \frac{1}{2n}f(0) + \frac{1}{n}\sum_{i=1}^{n-1} f\left(\frac{i}{n}\right) + \frac{1}{2n}f(1). \tag{1.5}$$

Such a rule is known to provide remarkably good approximations to the integral when f is smooth and periodic. This property of $T(f)$ follows by way of the Euler-Maclaurin expansion [3, p. 136]. Because the rectangle rule is good for smooth and periodic integrands, this has led in the past to the assumption for lattice rules that f is smooth and has period 1 in each of its s variables; that is,

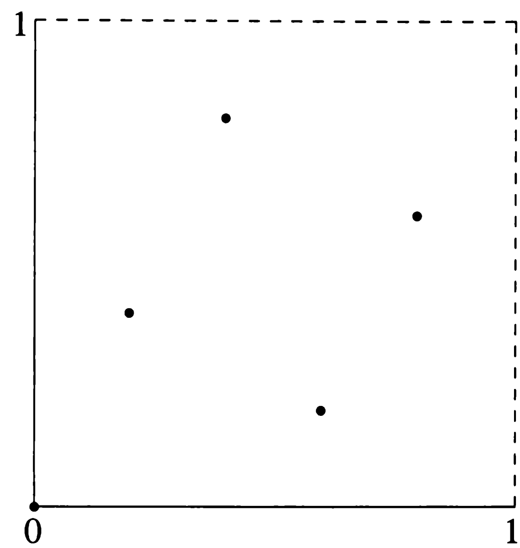
$$f(\mathbf{t}) = f(\mathbf{t}+\mathbf{z}), \quad \forall \mathbf{z} \in \mathbb{Z}^s \quad \text{and} \quad \forall \mathbf{t} \in \mathbb{R}^s.$$

An important property (as shown in [32]) of lattice rules is that they may be expressed as a multiple sum of the form

$$Q_\Lambda(f) = \frac{1}{d_1 d_2 \cdots d_t}\sum_{i_1=0}^{d_1-1}\sum_{i_2=0}^{d_2-1}\cdots\sum_{i_t=0}^{d_t-1} f\left(\left\{i_1\frac{\mathbf{z}_1}{d_1} + i_2\frac{\mathbf{z}_2}{d_2} + \cdots + i_t\frac{\mathbf{z}_t}{d_t}\right\}\right), \tag{1.6}$$

where the braces indicate that we take the fractional part of each component in the vector. For instance, $\{(\frac{5}{4}, \frac{4}{3}, \frac{1}{3})\} = (\frac{1}{4}, \frac{1}{3}, \frac{1}{3})$. The above form for a lattice rule may

Figure 1.1: The five points of a lattice rule.



be written in terms of two matrices. Suppose $D = \text{diag}\{d_1, d_2, \ldots, d_t\}$ and Z is a $t \times s$ integer matrix whose j-th row is $\mathbf{z}_j$. Then form (1.6) may be referred to as a t-cycle $D - Z$ form or simply a $D - Z$ form, and we denote it by

$$\mathcal{Q}[t, D, Z, s].$$

For a given lattice rule, there are many different representations of the form (1.6).

Example 1.1 *Consider the lattice rule given by*

$$\frac{1}{5}\sum_{i=0}^{4} f\left(\left\{i\frac{(1,2)}{5}\right\}\right). \tag{1.7}$$

The five quadrature points of this rule are

$$(0,0), \left(\tfrac{1}{5}, \tfrac{2}{5}\right), \left(\tfrac{2}{5}, \tfrac{4}{5}\right), \left(\tfrac{3}{5}, \tfrac{1}{5}\right), \left(\tfrac{4}{5}, \tfrac{3}{5}\right). \tag{1.8}$$

These points are shown in Figure 1.1. The same lattice rule may also be given by the formula

$$\frac{1}{5}\sum_{i=0}^{4} f\left(\left\{i\frac{(\ell,2\ell)}{5}\right\}\right) \quad \textit{for} \quad \ell = 2, 3, 4.$$

One may verify this by writing the quadrature points out and seeing that they are identical to those in (1.8).

Moreover, a $D-Z$ form of Q_Λ may be repetitive; that is, the order of the rule may be less than $\det D$. In this case it may be shown (as in [32]) that for some $k>1$ satisfying $k \mid \det D$,

$$\nu(Q_\Lambda) = \det D/k = d_1 d_2 \cdots d_t/k.$$

Example 1.2 *The lattice rule given in* (1.7) *has repetitive forms*

$$\frac{1}{10}\sum_{i=0}^{9} f\left(\left\{i\frac{(2,4)}{10}\right\}\right)$$

and

$$\frac{1}{25}\sum_{i_1=0}^{4}\sum_{i_2=0}^{4} f\left(\left\{i_1\frac{(1,2)}{5}+i_2\frac{(3,1)}{5}\right\}\right),$$

and of course there are many others. Upon writing the quadrature points, one sees that each quadrature point given in (1.8) *occurs twice in the first expression and five times in the second.*

Example 1.2 shows that a lattice rule may have many $D-Z$ forms. This problem of non-uniqueness of the $D-Z$ representation was partly solved by Sloan and Lyness [32]. They showed that every lattice rule has a non-repetitive r-cycle canonical form $Q[r, D, Z, s]$ in which the diagonal elements of D satisfy $d_{i+1} \mid d_i$, $1 \le i < r$, and $d_r > 1$. Their result is based on the fact that the set $\mathcal{A}(Q)$ of quadrature points form an abelian group under addition modulo $\mathbb{Z}^s$ (and also the fact that it may be decomposed into a direct sum of cyclic groups). The elements $d_1, \ldots, d_r$ are known as the invariants and the number r is known as the rank of the rule. Here, r and D are unique. The rank of a lattice rule, which may take any value between 1 and s inclusive, is in fact the minimum value of t required to write the lattice rule in the form (1.6). Sometimes it may be convenient to extend the r-cycle canonical form so that the rule has s invariants. This is done by including the trivial invariants $d_{r+1} = d_{r+2} = \cdots = d_s = 1$. These trivial invariants correspond to the trivial groups which contain the identity element. In the next section, we will look at some special classes of lattice rules that shall be of interest to us in this thesis.

1.2 Some special lattice rules

One special class of lattice rules that we shall be concerned with are those whose rank is 1. These rules are also known as number-theoretic rules and were introduced in works such as Korobov [15] and Hlawka [10]. We shall use this name throughout the thesis to refer to rank-1 lattice rules. They are given by

$$Q_{\mathrm{nt}}(f) = \frac{1}{n}\sum_{i=0}^{n-1} f\left(\left\{\frac{i\mathbf{z}}{n}\right\}\right), \tag{1.9}$$

where $\mathbf{z}$ is a suitably-chosen s-dimensional integer vector with no factor in common with n and the subscript "nt" is used to denote "number-theoretic". These rules are also known in the literature as good lattice point sets. A detailed account of these rules may be found in Niederreiter [23, 24]. An example of a number-theoretic rule with $n = 5$, $s = 2$ and $\mathbf{z} = (1, 2)$ is given in (1.7).

Another class of lattice rules that we shall consider in this thesis are those which are 2^s copies of the number-theoretic rule (1.9). Such rules are given by

$$Q_{\mathrm{c}}(f) = \frac{1}{2^s n}\sum_{i=0}^{n-1}\sum_{k_1=0}^{1}\cdots\sum_{k_s=0}^{1} f\left(\frac{1}{2}\left\{\frac{i\mathbf{z}}{n}\right\} + \frac{(k_1, k_2, \ldots, k_s)}{2}\right),$$

where n is an odd number and $\mathbf{z}$ is an integer vector. (In general, it is possible to have ℓ^s copy rules; here, we are concerned with the case $\ell = 2$.) These are maximal rank lattice rules (they have a rank equal to s) and may be obtained by subdividing the unit cube $[0, 1]^s$ into 2^s smaller cubes each with sides of length $\frac{1}{2}$, and then applying an appropriately scaled version of the rule to each smaller cube. For more information about these rules, one may refer to [6].

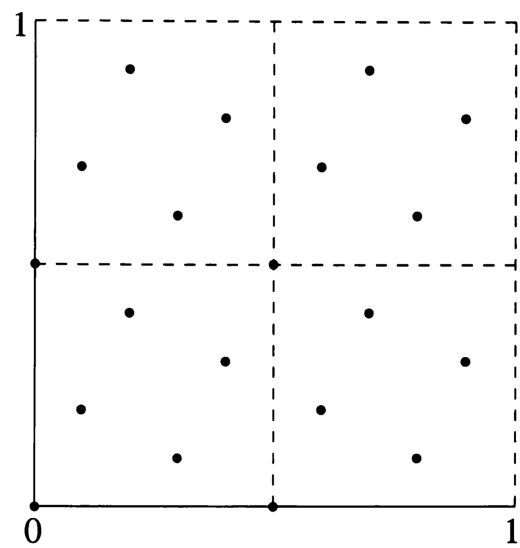
Example 1.3 *The* 2^2 *copy of the five-point lattice rule* (1.7) *is given by*

$$\begin{aligned}
&\frac{1}{2^2\times 5}\sum_{i=0}^{4}\sum_{k_1=0}^{1}\sum_{k_2=0}^{1} f\left(\frac{1}{2}\left\{\frac{i(1,2)}{5}\right\} + \frac{(k_1,k_2)}{2}\right)\\
&= \frac{1}{20}\sum_{i=0}^{4}\sum_{k_1=0}^{1}\sum_{k_2=0}^{1} f\left(\left\{i\frac{(1,2)}{10} + \frac{(k_1,k_2)}{2}\right\}\right).
\end{aligned}$$

The points of this rule are shown in Figure 1.2.

In this thesis, we shall also consider lattice rules that are known as projection-regular rules. In order to define them, we start with the projections of a lattice

Figure 1.2: A 2^2 copy of a five-point lattice rule.



rule. For $1 \leq \ell \leq s$, a ℓ-dimensional projection of a lattice rule, defined over $[0, 1)^s$, is the ℓ-dimensional rule obtained when all of specified $(s - \ell)$ components of each quadrature point is omitted. As a special case, if the last $(s - \ell)$ components are omitted, then the resulting rule will be referred to as the principal projection of the original rule. These ℓ-dimensional projections are also lattice rules. An s-dimensional lattice rule Q_Λ having invariants $d_1, d_2, \ldots, d_s$, is said to be projection-regular if for $1 \leq \ell \leq s$, the principal projections have order $d_1 d_2 \cdots d_\ell$. In other words, projection-regular lattice rules are those in which all the principal projections have the maximum possible order.

In a canonical form $Q[r, D, Z, s]$ of a lattice rule, as mentioned earlier, r and D are unique. However, there remain many possibilities for Z. Except for the case of projection-regular (see [33]) and prime-power (see [16]) rules, no such unique Z is known. The unique $D - Z$ form for prime-power rules is called an ultratriangular form in [16] . Each ultratriangular form has a set of column indices associated with it. In Chapter 2 we shall extend the class of unique representations by using the fact that every lattice rule may be decomposed into its Sylow p-components. These components are prime-power rules, each of which has a unique ultratriangular form.

By reassembling these ultratriangular forms in a defined way, it is possible to obtain a canonical form for any lattice rule. A special case occurs when the ultratriangular forms for each of the Sylow p-components have a consistent set of column indices. We shall find a unique form for such rules. Moreover, we also give an application of the ultratriangular form for prime-power rules. For a given set of column indices and invariants, we obtain a formula for the number of ultratriangular forms, and hence the number of prime-power lattice rules, having these column indices and invariants.

For any given s-dimensional lattice Λ, there exists a set of s generators $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_s$ such that each point of the lattice may be written in terms of these generators; that is,

$$\mathbf{p} = \sum_{i=1}^{s} \lambda_i \mathbf{a}_i, \qquad \lambda_i \in \mathbb{Z}.$$

Associated with the set of generators is a generator matrix A. This is an $s \times s$ matrix whose j-th row is $\mathbf{a}_j$ for $1 \leq j \leq s$. Corresponding to the lattice Λ for a lattice rule is its dual denoted by $\Lambda^{\perp}$ and defined in the following way.

Definition 1.1 *A dual lattice $\Lambda^{\perp}$ of an integration lattice Λ comprises all $\mathbf{h} \in \mathbb{Z}^s$ such that*

$$\mathbf{h} \cdot \mathbf{t} \in \mathbb{Z}, \quad \forall \mathbf{t} \in \Lambda,$$

where $\mathbf{h} \cdot \mathbf{t} = h_1 t_1 + \cdots + h_s t_s$ is the normal dot product in $\mathbb{R}^s$.

The dual lattice plays a very important role in the error analysis of lattice rules (see (1.13) in Section 1.4) and it may be specified by an $s \times s$ generator matrix $B = (A^T)^{-1}$. This matrix B is an integer matrix which may be written in a unique upper triangular form. This unique form for integer matrices is known in the literature as the Hermite normal form (see for example, [30]). All the theory based on this generator matrix for $\Lambda^{\perp}$ has made the assumption that the Hermite normal form is upper triangular. However, results concerning the unique Z for lattice rules having a consistent set of column indices, in Chapter 2, indicate that a lower triangular Hermite normal form might be appropriate for study. In Chapter 3 we look at such representations of B for the special case of projection-regular rules. The results obtained give conditions on the lower triangular generator matrix which allow a projection-regular rule to be easily recognized.

1.3 Vertex-modified number-theoretic rules

Suppose the rule (1.2) is such that $\mathbf{t}_0 = \mathbf{0}$ and that all the other quadrature points $\mathbf{t}_1, \ldots, \mathbf{t}_{n-1}$ belong to the half-open unit cube $[0,1)^s$. If the integrand f is periodic with period 1 in each of its s variables, then it might make sense to use this equal-weight rule in which no components of the quadrature points are 1 since such an element may always be replaced by 0. However, if the integrand is not 1-periodic in each variable, then it might be better to modify the equal-weight rule so that all the 2^s vertices of $[0,1]^s$ are used as quadrature points. In [25] Niederreiter and Sloan proposed such a rule. Their modified rule is given by

$$M(f) = \sum_{i_1=0}^{1} \cdots \sum_{i_s=0}^{1} w_{i_1,\ldots,i_s} f(i_1, \ldots, i_s) + \frac{1}{n} \sum_{i=1}^{n-1} f(\mathbf{t}_i), \tag{1.10}$$

where the weights $w_{i_1,\ldots,i_s}$ corresponding to the vertices $(i_1, \ldots, i_s)$ are such that their sum is $1/n$. For this rule there are obviously many choices for the weights $w_{i_1,\ldots,i_s}$. However, Niederreiter and Sloan [25] showed that the weights may be chosen optimally in the sense that its discrepancy (to be defined in Section 5.2) is minimized. When this is the case the resulting rule will be referred to as the optimal vertex-modified rule.

For non-periodic integrands, we may also modify Q_{nt}, given in (1.9), in a manner analogous to (1.10) to get the vertex-modified number-theoretic rule

$$M_{\mathrm{nt}}(f) = \sum_{i_1=0}^{1} \cdots \sum_{i_s=0}^{1} w_{i_1,\ldots,i_s} f(i_1, \ldots, i_s) + \frac{1}{n} \sum_{i=1}^{n-1} f\left(\left\{\frac{i\mathbf{z}}{n}\right\}\right). \tag{1.11}$$

We remark that if f is 1-periodic in each of its s variables, then the value of $M_{\mathrm{nt}}(f)$ is the same as the value of $Q_{\mathrm{nt}}(f)$. If the weights are chosen optimally in rule (1.11), then we have what we term the optimal vertex-modified number-theoretic rule.

1.4 Error in a lattice rule

How well one lattice rule performs with respect to another is determined by its error in the approximation of the integral (1.1). In this section, we discuss two error criteria that have been used in the analysis of lattice rules.

In order to study the first one, namely P_α, we assume that f has the absolutely convergent Fourier series representation

$$f(\mathbf{t}) = \sum_{\mathbf{h}\in\mathbb{Z}^s} \hat{f}(\mathbf{h}) e^{2\pi i \mathbf{h}\cdot\mathbf{t}}, \tag{1.12}$$

where

$$\hat{f}(\mathbf{h}) = \int_{[0,1]^s} e^{-2\pi i \mathbf{h}\cdot\mathbf{t}} f(\mathbf{t})\,\mathrm{d}\mathbf{t}, \quad \mathbf{h} \in \mathbb{Z}^s.$$

Necessarily, f is 1-periodic in each of its s variables. Now applying the lattice rule Q_Λ, given in (1.3), to the series (1.12), we get

$$Q_\Lambda(f) = \sum_{\mathbf{h}\in\mathbb{Z}^s} \hat{f}(\mathbf{h}) Q_\Lambda\left(e^{2\pi i \mathbf{h}\cdot\mathbf{t}}\right) = \sum_{\mathbf{h}\in\Lambda^\perp} \hat{f}(\mathbf{h}),$$

where $\Lambda^\perp$ is the dual lattice of Λ and the last step above follows (as shown in [31]) by using

$$Q_\Lambda\left(e^{2\pi i \mathbf{h}\cdot\mathbf{t}}\right) = \begin{cases} 1, & \mathbf{h} \in \Lambda^\perp, \\ 0, & \text{otherwise.} \end{cases}$$

It then follows that for a rule Q_Λ with f having an absolutely convergent Fourier series, the error $Q_\Lambda(f) - I(f)$ is given by

$$\begin{aligned} Q_\Lambda(f) - I(f) &= \sum_{\mathbf{h}\in\Lambda^\perp} \hat{f}(\mathbf{h}) - \int_{[0,1]^s} f(\mathbf{t})\,\mathrm{d}\mathbf{t} \\ &= \sum_{\mathbf{h}\in\Lambda^\perp} \hat{f}(\mathbf{h}) - \hat{f}(\mathbf{0}) = {\sum_{\mathbf{h}\in\Lambda^\perp}}' \hat{f}(\mathbf{h}), \end{aligned} \tag{1.13}$$

where the prime on the sum indicates that the $\mathbf{h} = \mathbf{0}$ term is to be omitted.

In order to have a bound for this error, we consider the classes of functions whose Fourier coefficients decay sufficiently rapidly. For $\alpha > 1$ and $K > 0$, let $C_\alpha(K)$ be a set of periodic integrands defined by

$$C_\alpha(K) := \left\{ f : |\hat{f}(\mathbf{h})| \le \frac{K}{(\bar{h}_1\bar{h}_2\cdots\bar{h}_s)^\alpha} \right\},$$

where $\bar{h}_j = \max(|h_j|, 1)$. The error bound is then given in the following definition.

Definition 1.2 *For f belonging to the class $C_\alpha(K)$, the error in a lattice rule Q_Λ satisfies the inequality*

$$|Q_\Lambda(f) - I(f)| \leq K P_\alpha(Q_\Lambda),$$

where

$$P_\alpha(Q_\Lambda) := \sum_{\mathbf{h}\in\Lambda^\perp}{}' \frac{1}{(\bar{h}_1 \bar{h}_2 \cdots \bar{h}_s)^\alpha}. \tag{1.14}$$

In order to compare the potential of different classes of lattice rules, the average of the quantity $P_\alpha(Q_\Lambda)$ has been used (see [4] and [5]). For the number-theoretic rule given in (1.9), this average is defined in the following way.

Definition 1.3 *For any integer $n \geq 2$, let $X = X(n)$ be the set of all $\mathbf{z} \in \mathbb{Z}^s$ whose components z_j are relatively prime to n and satisfy $1 \leq z_j \leq n-1$. The average of $P_\alpha(Q_{\mathrm{nt}})$ for number-theoretic rules, over $\mathbf{z} \in X$ is*

$$E_n[P_\alpha(Q_{\mathrm{nt}})] := \frac{1}{\varphi(n)^s} \sum_{\mathbf{z}\in X} P_\alpha(Q_{\mathrm{nt}}),$$

where φ is Euler's function (that is, $\varphi(n)$ is the number of positive integers less than n which are relatively prime to n).

Since $E_n[P_\alpha(Q_{\mathrm{nt}})]$ is an average of $P_\alpha(Q_{\mathrm{nt}})$ over a set X, there must exist at least one $\mathbf{z}$ in the set for which

$$P_\alpha(Q_{\mathrm{nt}}) \leq E_n[P_\alpha(Q_{\mathrm{nt}})].$$

Another criterion that has previously been used to assess the performance of lattice rules is the quantity $R(Q_\Lambda)$ defined by

$$R(Q_\Lambda) := \sum_{\substack{\mathbf{h}\in\Lambda^\perp \\ \mathbf{h}\in W(n)}}{}' \frac{1}{\bar{h}_1 \bar{h}_2 \cdots \bar{h}_s}, \tag{1.15}$$

where $W(n) = \{\mathbf{h} \in \mathbb{Z}^s : \frac{-n}{2} < h_k \leq \frac{n}{2}, 1 \leq k \leq s\}$.

When the integrands are periodic, P_α and R are usually considered as suitable figures of merit for lattice rules. In the next section, we look at error bounds that apply to more general rules and to integrands which are not necessarily periodic.

1.5 Error in a general quasi-Monte Carlo rule

Error bounds for quasi-Monte Carlo integration are based on various measures of the uniformity of distribution of the point sets. One such measure is the L_2 discrepancy, which we shall denote by $D(Q)$. This quantity appears in the error bound given by

$$|I(f) - Q(f)| \leq D(Q)V(f), \tag{1.16}$$

where $V(f)$ is a measure of variation of the integrand f in the sense of Hardy and Krause. The quantity $D(Q)$ has previously been derived by using two different techniques. One of them is based on the Koksma-Hlawka inequality [38] (since the error bound (1.16) corresponds to the L_2 version of this inequality) and the other is based on the use of reproducing kernel Hilbert spaces. We present both these methods for deriving $D(Q)$ in Chapter 4. We shall also give in Chapter 4 an analogue of the error bound (1.16) for periodic integrands.

How well a class of Monte Carlo rules Q performs for non-periodic integrands may be measured by using the average of $D^2(Q)$. An expression for this average may be derived for various classes of rules and their values then compared with averages or expected values for other classes of rules with approximately the same number of points. The average discrepancy that we shall use is analogous to the one given in Definition 1.3. For number-theoretic rules, it is defined in the following way.

Definition 1.4 *For any integer $n \geq 2$, let $X = X(n)$ be the set of all $\mathbf{z} \in \mathbb{Z}^s$ whose components z_j are relatively prime to n and satisfy $1 \leq z_j \leq n-1$. The average of the squared discrepancy $D^2(Q_{\rm nt})$ for number-theoretic rules, over $\mathbf{z} \in X$ is*

$$E_n[D^2(Q_{\rm nt})] := \frac{1}{\varphi(n)^s} \sum_{\mathbf{z} \in X} D^2(Q_{\rm nt}).$$

In an analogous way the average squared discrepancy for optimal vertex-modified number-theoretic and 2^s copy rules may be defined.

For non-periodic integrands, Joe [13] gave numerical evidence that values of the average L_2 discrepancy for number-theoretic rules are smaller than the expected values for Monte Carlo rules when the dimension s is less than 18. We shall carry out similar comparisons of the averages for certain classes of rules (to be named below) in chapters 5, 6 and 7.

In Chapter 5, we obtain an expression for the average of the squared L_2 discrepancy for optimal vertex-modified number-theoretic rules. Values of this average are then compared with the corresponding average for normal number-theoretic rules and the expected value for Monte Carlo rules.

In the case of periodic integrands, it has previously been established that the average (compare Definition 1.3) of the quantity P_α and the values of R for 2^s copy rules are better than those for number-theoretic rules with roughly the same number of points. In the case when the integrand is not periodic no such comparison has been done previously and we shall do this in Chapter 6.

As mentioned earlier, quantities P_α and R have been used to study error in the case of periodic integrands. It might be useful to consider an analogue of the L_2 discrepancy to study the error for such periodic integrands. In Chapter 7, we shall consider this problem.

Chapter 2

Ultratriangular form for prime-power lattice rules

2.1 Chapter summary

In this chapter, we shall extend the class of unique representations for lattice rules by making use of the fact that any lattice rule may be expressed as a sum of prime-power rules. This is done in Section 2.4 where we treat a special class of lattice rules in which all the prime-power component rules have a consistent set of column indices in their ultratriangular form. For this class we obtain a unique $D-Z$ representation. In this unique form, Z is a column-permuted unit upper triangular matrix and has some of the properties inherited from the ultratriangular forms of its component rules. In the section that follows we give some required definitions and results as well as some properties of prime-power lattice rules. In Section 2.3 we present the theory behind decomposition of a general lattice rule into prime-power rules and their appropriate reassembly to obtain a canonical form for a general lattice rule. In the final section, Section 2.5, an application of the ultratriangular form is given. We use it to obtain a formula for calculating the number of prime-power rules having a given set of invariants and column indices. The results of this chapter have appeared in Reddy and Joe [28].

2.2 Background material

In order to construct our unique $D-Z$ form from any given $D-Z$ form, we shall use certain transformations which leave the lattice rule unchanged. The transformations required in this chapter are taken from [16] and given in the following theorem.

Theorem 2.1 *The rule* $Q_\Lambda = Q[t, D, Z, s]$ *given by*

$$Q_\Lambda(f) = \frac{1}{d_1 d_2 \cdots d_t} \sum_{i_1=0}^{d_1-1} \sum_{i_2=0}^{d_2-1} \cdots \sum_{i_t=0}^{d_t-1} f\left(\left\{i_1\frac{\mathbf{z}_1}{d_1} + i_2\frac{\mathbf{z}_2}{d_2} + \cdots + i_t\frac{\mathbf{z}_t}{d_t}\right\}\right), \tag{2.1}$$

is unaltered if Z is modified by applying one of the following transformations, or a sequence of them.

(a) *Replace* $\mathbf{z}_i$ *by* $\ell\mathbf{z}_i$ *for* $\ell \in \mathbb{Z}$ *satisfying* $\gcd(\ell, d_i) = 1$.

(b) *Replace* $\mathbf{z}_i$ *by* $\mathbf{z}_i + d_i\mathbf{x}$ *for* $\mathbf{x} \in \mathbb{Z}^s$.

(c) *Replace* $\mathbf{z}_i$ *by* $\mathbf{z}_i + (md_i/d_j)\mathbf{z}_j$ *for* $j \neq i$, $m \in \mathbb{Z}$, *and* $d_j \mid md_i$.

A full list of transformations may be found in [16]. In this chapter we shall need one further transformation. This is given in Lemma 2.5 of the following section.

We now consider lattice rules of prime-power order or simply, prime-power rules. Lyness and Joe [16] have developed a unique canonical form, the ultratriangular form, for such rules. This unique form is based on a column-permuted version of an upper triangular matrix and plays a crucial role in the development of new results in this chapter.

Definition 2.2 *The $t \times s$ matrix Z is termed column permuted unit upper triangular (cpuut) if and only if there exist distinct column indices $\eta_1, \eta_2, \ldots, \eta_{\min(t,s)}$, where $\eta_j \in \{1, 2, \ldots, s\}$, and*

$$z_{k,\eta_j} = \begin{cases} 1, & \textit{when } k = j, \\ 0, & \textit{when } k > j, \end{cases} \qquad 1 \leq j \leq \min(t, s).$$

A column permuted unit upper triangular matrix Z may be written in terms of a unit upper triangular matrix Z' as $Z' = ZP$, where P is an $s \times s$ permutation matrix whose j-th column has a 1 in the η_j-th position for $1 \leq j \leq s$. Note that the unassigned column indices from $\{1, 2, \ldots, s\}$ are arbitrarily assigned to the rest of the columns.

The unique ultratriangular form for a prime-power rule having order p^β, for some prime p, is then defined as follows.

Definition 2.3 *An ultratriangular $D - Z$ form for a prime-power rule is one in which*

(a) $t \leq s$,

(b) *the diagonal elements of D satisfy*

$$d_1 \geq d_2 \geq \cdots \geq d_t > 1,$$

(c) d_i *and the components of* $\mathbf{z}_i = (z_{i1}, \ldots, z_{is})$ *satisfy* $\gcd(z_{i1}, \ldots, z_{is}, d_i) = 1$ *and* $\mathbf{z}_i/d_i \in [0, 1)^s$,

(d) Z *is cpuut with column indices* $\eta_1, \eta_2, \ldots, \eta_t$,

(e) $z_{j,k}/p \in \mathbb{Z}$ *for* $1 \leq k < \eta_j$,

(f) *if* $d_j = d_{j+1}$, *then* $\eta_j < \eta_{j+1}$,

(g) $0 \leq z_{k,\eta_j} < d_k/d_j$, $k \neq j$.

Given a $D-Z$ form for a prime-power rule, the ultratriangular form may be obtained by using certain transformations, some of which are given in Theorem 2.1. The full details may be found in [16]. This form for a prime-power rule is a canonical form with rank t and invariants $d_1, d_2, \ldots, d_t$.

Example 2.1 *Consider the Z-matrix,*

$$Z = \begin{bmatrix} 1 & \mathsf{f}_1 & \mathsf{c}_1 & \mathsf{f}_2 & \mathsf{f}_3 & \mathsf{f}_4 \\ 0 & \mathsf{b}_1 & \mathsf{d}_1 & \mathsf{b}_2 & \mathsf{b}_3 & 1 \\ 0 & \mathsf{b}_4 & \mathsf{d}_2 & 1 & \mathsf{f}_5 & 0 \\ 0 & 1 & \mathsf{c}_2 & 0 & \mathsf{f}_6 & 0 \\ 0 & 0 & \mathsf{d}_3 & 0 & 1 & 0 \end{bmatrix},$$

where the $\mathsf{b}_j, 1 \le j \le 4, \mathsf{c}_k, 1 \le k \le 2, \mathsf{d}_\ell, 1 \le \ell \le 3$ *and* $\mathsf{f}_m, 1 \le m \le 6$, *represent integers. This is a* 5×6 *cpuut matrix with column indices given by* $1, 6, 4, 2, 5$. *Here the integers denoted by* d_ℓ *should satisfy condition (e), but not necessarily condition (g) of the above definition; the integers denoted by* f_m *need to satisfy (g), but not necessarily (e); whereas the integers denoted by* b_j *should satisfy both of the conditions (e) and (g). Condition (c) of the above definition ensures that the integer values in the i-th row belong to* $[0, d_i)$. *In particular, the remaining integers* c_1 *and* c_2 *should satisfy* $0 \le \mathsf{c}_1 < d_1$ *and* $0 \le \mathsf{c}_2 < d_4$. *Moreover, condition (f) of the above definition requires that* $d_3 \ne d_2$ *and* $d_4 \ne d_3$. *Hence, we have* $d_1 \ge d_2 > d_3 > d_4 \ge d_5$.

For this Z-matrix the permutation matrix P is

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and the unit upper triangular matrix $Z' = ZP$ *is given by*

$$\begin{bmatrix} 1 & \mathsf{f}_4 & \mathsf{f}_2 & \mathsf{f}_1 & \mathsf{f}_3 & \mathsf{c}_1 \\ 0 & 1 & \mathsf{b}_2 & \mathsf{b}_1 & \mathsf{b}_3 & \mathsf{d}_1 \\ 0 & 0 & 1 & \mathsf{b}_4 & \mathsf{f}_5 & \mathsf{d}_2 \\ 0 & 0 & 0 & 1 & \mathsf{f}_6 & \mathsf{c}_2 \\ 0 & 0 & 0 & 0 & 1 & \mathsf{d}_3 \end{bmatrix}.$$

2.3 Decomposition and reassembly of lattice rules

The results of this section are based on the group structure of $\mathcal{A}(Q)$. However, we shall not be concerned with this aspect of the theory here. We start this section with the sum of two lattice rules. This is a very simple but important concept.

Definition 2.4 *Suppose $Q_{\Lambda,1}$ and $Q_{\Lambda,2}$ are two s-dimensional lattice rules. If*

$$Q_{\Lambda,1}(f) = \frac{1}{N_1} \sum_{j=0}^{N_1-1} f(\mathbf{x}_j) \text{ and } Q_{\Lambda,2}(f) = \frac{1}{N_2} \sum_{k=0}^{N_2-1} f(\mathbf{y}_k), \tag{2.2}$$

where $\mathbf{x}_j, \mathbf{y}_k \in [0,1)^s$, then their sum Q_Λ, written as $Q_{\Lambda,1}+Q_{\Lambda,2}$, is the s-dimensional lattice rule given by

$$Q_\Lambda(f) = (Q_{\Lambda,1} + Q_{\Lambda,2})(f) = \frac{1}{N_1 N_2} \sum_{j=0}^{N_1-1} \sum_{k=0}^{N_2-1} f(\{\mathbf{x}_j + \mathbf{y}_k\}). \tag{2.3}$$

We have $\nu(Q_{\Lambda,1} + Q_{\Lambda,2}) \le \nu(Q_{\Lambda,1})\nu(Q_{\Lambda,2})$ with equality being valid if $\nu(Q_{\Lambda,1})$ and $\nu(Q_{\Lambda,2})$ are relatively prime (see [31, pp. 54–56]).

If $Q_{\Lambda,1} = \mathcal{Q}[t_1, D_1, Z_1, s]$ and $Q_{\Lambda,2} = \mathcal{Q}[t_2, D_2, Z_2, s]$, then it is not difficult to show from (2.1), (2.2), and (2.3) that a $D-Z$ form for the sum of $Q_{\Lambda,1}$ and $Q_{\Lambda,2}$ is given by $\mathcal{Q}[t_3, D_3, Z_3, s]$, where $t_3 = t_1 + t_2$, $D_3 = \operatorname{diag}\{D_1, D_2\}$, and

$$Z_3 = \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix}.$$

Thus we write

$$\mathcal{Q}[t_3, D_3, Z_3, s] = \mathcal{Q}[t_1, D_1, Z_1, s] + \mathcal{Q}[t_2, D_2, Z_2, s].$$

The following lemma gives another transformation that we shall need in this chapter. This follows from the discussion in [31, p. 51].

Lemma 2.5 *When m and n are relatively prime,*

$$\mathcal{Q}[1, m, \mathbf{z}, s] + \mathcal{Q}[1, n, \mathbf{z}', s] = \mathcal{Q}[1, mn, m\mathbf{z}' + n\mathbf{z}, s]. \tag{2.4}$$

Suppose we have a $D-Z$ form with $\det D$ having prime factorization

$$\det D = \prod_{i=1}^{t} d_i = p_1^{\beta_1} p_2^{\beta_2} \cdots p_q^{\beta_q}$$

with the prime factorization of individual elements d_i given by

$$d_i = p_1^{\beta_{1,i}} p_2^{\beta_{2,i}} \cdots p_q^{\beta_{q,i}} \quad \text{with} \quad \sum_{i=1}^{t} \beta_{j,i} = \beta_j, \quad 1 \le j \le q.$$

(Some values of $\beta_{j,i}$ may be zero.) If we let $\bar{d}_i^{(k)}$ denote the prime p_k-component of d_i; that is, $\bar{d}_i^{(k)} = p_k^{\beta_{k,i}}$, then it is shown in [17] that the lattice rule $Q_\Lambda = \mathcal{Q}[t, D, Z, s]$ may be decomposed as

$$Q_\Lambda = P^{(1)} + P^{(2)} + \cdots + P^{(q)},$$

where $P^{(k)} = \mathcal{Q}[t, \bar{D}^{(k)}, Z, s]$. Here $\bar{D}^{(k)}$ is the $t \times t$ diagonal matrix having elements $\bar{d}_i^{(k)}$. The prime-power rule $P^{(k)}$ is known as the Sylow p_k-component of the original rule $Q_\Lambda = \mathcal{Q}[t, D, Z, s]$. Hence a general lattice rule may be decomposed into the sum of its Sylow p_k-components.

Let $C^{(k)}$ denote a canonical form of $P^{(k)}$ with rank and invariants

$$r^{(k)}; \quad d_1^{(k)}, d_2^{(k)}, \ldots, d_{r^{(k)}}^{(k)};$$

that is,

$$C^{(k)} = \mathcal{Q}[r^{(k)}, D^{(k)}, Z^{(k)}, s], \tag{2.5}$$

where $D^{(k)} = \operatorname{diag}\{d_1^{(k)}, d_2^{(k)}, \ldots, d_{r^{(k)}}^{(k)}\}$ and $Z^{(k)}$ is a Z-matrix for this canonical form. We then have the following result.

Theorem 2.6 *Suppose the lattice rule Q_Λ may be expressed as the (direct) sum*

$$Q_\Lambda = C^{(1)} + C^{(2)} + \cdots + C^{(q)},$$

where $C^{(k)}$, given by (2.5), is a canonical form for the Sylow p_k-component of Q_Λ. Then Q_Λ has a canonical $D - Z$ form $\mathcal{Q}[r, D, Z, s]$, where

$$r = \max(r^{(1)}, r^{(2)}, \ldots, r^{(q)}), \tag{2.6}$$

and

$$d_i = \prod_{k=1}^{q} d_i^{(k)}, \quad \mathbf{z}_i = \sum_{k=1}^{q} \left(\prod_{\substack{j=1 \\ j \neq k}}^{q} d_i^{(j)} \right) \mathbf{z}_i^{(k)}, \quad 1 \leq i \leq r. \tag{2.7}$$

Proof. The fact that Q_Λ has a canonical $D - Z$ form $\mathcal{Q}[r, D, Z, s]$ with r and d_i as given in (2.6) and (2.7), respectively, follows from [17]. The expression for $\mathbf{z}_i$ in (2.7) may be obtained by repeated application of the transformation given in (2.4).

□

Note in (2.6) and (2.7) that if there is a value of $r^{(k)}$ less than r, then we need values of $d^{(k)}_{r^{(k)}+1}, \ldots, d^{(k)}_r$ and $\mathbf{z}^{(k)}_{r^{(k)}+1}, \ldots, \mathbf{z}^{(k)}_r$. To obtain these values, we use the trivial invariants $d^{(k)}_{r^{(k)}+1} = \cdots = d^{(k)}_r = 1$ and arbitrarily take the vectors $\mathbf{z}^{(k)}_{r^{(k)}+1}, \ldots, \mathbf{z}^{(k)}_r$ to be zero vectors.

Example 2.2 *Consider the $D - Z$ form of a lattice rule given by*

$$D = \begin{bmatrix} 2^2 \times 3^2 \times 5^2 & 0 \\ 0 & 2 \times 3 \times 5 \end{bmatrix}, \quad Z = \begin{bmatrix} 321 & 38 & 747 \\ 7 & 24 & 11 \end{bmatrix}. \tag{2.8}$$

Here we take $p_1 = 2$, $p_2 = 3$, and $p_3 = 5$. We first write Q_Λ as a sum of its Sylow p_k-components, that is, $Q_\Lambda = P^{(1)} + P^{(2)} + P^{(3)}$, where $P^{(k)} = Q[t, \bar{D}^{(k)}, Z, s]$ with $t = 2, s = 3$, and

$$\bar{D}^{(1)} = \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix}, \quad \bar{D}^{(2)} = \begin{bmatrix} 9 & 0 \\ 0 & 3 \end{bmatrix}, \quad \bar{D}^{(3)} = \begin{bmatrix} 25 & 0 \\ 0 & 5 \end{bmatrix}.$$

Now we need a canonical form for each Sylow p_k-component which we shall take to be the unique ultratriangular form. We write $U^{(k)}$ for the ultratriangular form of the Sylow p_k-component. Associated with each $U^{(k)}$ are its $r^{(k)}$ column indices (see Definition 2.2) which we denote by $\eta^{(k)}_1, \eta^{(k)}_2, \ldots, \eta^{(k)}_{r^{(k)}}$. Using the procedure given in [16] we find that $Q_\Lambda = U^{(1)} + U^{(2)} + U^{(3)}$, where $U^{(k)} = Q[r^{(k)}, D^{(k)}, Z^{(k)}, s]$ with $r^{(1)} = 1$, $r^{(2)} = r^{(3)} = 2$, and

$$D^{(1)} = [\ 4\ ], \quad Z^{(1)} = [\ 1 \ \ 2 \ \ 3\ ],$$

$$D^{(2)} = \begin{bmatrix} 9 & 0 \\ 0 & 3 \end{bmatrix}, \quad Z^{(2)} = \begin{bmatrix} 0 & 1 & 3 \\ 1 & 0 & 2 \end{bmatrix}, \quad D^{(3)} = \begin{bmatrix} 25 & 0 \\ 0 & 5 \end{bmatrix}, \quad Z^{(3)} = \begin{bmatrix} 1 & 3 & 7 \\ 0 & 1 & 4 \end{bmatrix}.$$

The column indices for $U^{(1)}$, $U^{(2)}$, and $U^{(3)}$ are given by $\eta^{(1)}_1 = 1$; $\eta^{(2)}_1 = 2$, $\eta^{(2)}_2 = 1$; and $\eta^{(3)}_1 = 1$, $\eta^{(3)}_2 = 2$, respectively. Note that the determinant of the matrix D in (2.8) *is* 27,000, *while*

$$\det D^{(1)} \times \det D^{(2)} \times \det D^{(3)} = 13{,}500 < \det D.$$

Hence the original $D - Z$ form cannot be a canonical form since it was repetitive.

Following the procedure given in Theorem 2.6, we obtain a canonical form for the lattice rule specified by (2.8). *The rule has rank* 2 *with the* $D-Z$ *form given by*

$$D = \begin{bmatrix} 900 & 0 \\ 0 & 15 \end{bmatrix}, \quad Z = \begin{bmatrix} 261 & 658 & 1227 \\ 5 & 3 & 22 \end{bmatrix}. \tag{2.9}$$

By using Theorem 2.1(b), this Z-matrix may be replaced by

$$Z = \begin{bmatrix} 261 & 658 & 327 \\ 5 & 3 & 7 \end{bmatrix}.$$

2.4 Unique form when the Sylow p-components in ultratriangular form have a consistent set of column indices

In this section we consider the canonical form obtained from Theorem 2.6 when the canonical forms for all the Sylow p_k-components are ultratriangular forms. We shall see that we can obtain a unique canonical form when the column indices for these ultratriangular forms are consistent (to be defined below).

Recalling from the previous section that $r = \max(r^{(1)}, r^{(2)}, \dots, r^{(q)})$, it is clear that there exists an ℓ, $1 \le \ell \le q$ such that $r^{(\ell)} = r$. Now let the column indices for the corresponding ultratriangular form $U^{(\ell)}$ be denoted by $\eta_1, \dots, \eta_r$. Then we say that the column indices of the ultratriangular forms for the Sylow p_k-components are consistent when for $1 \le k \le q$,

$$\eta_j^{(k)} = \eta_j, \quad 1 \le j \le r^{(k)}.$$

We shall assume that this is the situation throughout this section.

Since the column indices are consistent, then all the $\mathbf{z}_i^{(k)}$, $1 \le k \le q$, $1 \le i \le r$, have zeros in positions $\eta_1, \dots, \eta_{i-1}$. It follows from (2.7) that $\mathbf{z}_i$ has zeros in the same positions. Moreover, the η_i-th component of $\mathbf{z}_i$ is given by

$$\sum_{k=1}^{q} \left(\prod_{\substack{j=1 \\ j \ne k}}^{q} d_i^{(j)} \right) = \sum_{k=1}^{q} (d_i / d_i^{(k)}). \tag{2.10}$$

(Note that for values of m for which $r^{(m)} < r$, we arbitrarily took the vectors $\mathbf{z}^{(m)}_{r^{(m)}+1}, \ldots, \mathbf{z}^{(m)}_r$ to be zero vectors. Thus for $r^{(m)} < i \leq r$, $\mathbf{z}_i$ in (2.7) would be missing the $k = m$ term for those values of m for which $r^{(m)} < r$.) Since each of the terms in the last sum in (2.10) is missing a (prime) factor $d_i^{(k)}$, it is clear that the η_i-th component of $\mathbf{z}_i$ is relatively prime to d_i. Elementary number theory then shows there exists $\lambda_i \in \mathbb{Z}$ such that

$$\lambda_i \sum_{k=1}^{q} (d_i/d_i^{(k)}) \equiv 1 \pmod{d_i}.$$

Using Theorem 2.1(a), we can multiply $\mathbf{z}_i$ by λ_i and we see from Theorem 2.1(b) that the η_i-th component of $\mathbf{z}_i$ may be replaced with a 1. Note that in these transformations of $\mathbf{z}_i$, any zero components are preserved. This leads to the following lemma.

Lemma 2.7 *If the column indices for the ultratriangular forms of its Sylow p-components are consistent, then Q_Λ may be expressed in a canonical form in which Z is cpuut (see Definition 2.2) with column indices $\eta_1, \ldots, \eta_r$.*

If the column indices for the ultratriangular forms are not consistent, then there is no guarantee that the Z-matrix can be made cpuut. This is evidenced by the example at the end of the previous section in which the Z-matrix was given in (2.9).

In order to show that it is possible to obtain a unique $D-Z$ form, it is convenient to pad out the canonical r-cycle form to an s-cycle form. To do this, we take $d_{r+1} = \cdots = d_s = 1$. Moreover, we note that there are $s - r$ values in $\{1, 2, \ldots, s\}$ which are not assigned to be column indices. We now take $\eta_{r+1}, \ldots, \eta_s$ to be these $s - r$ unassigned values such that

$$\eta_{r+1} < \eta_{r+2} < \cdots < \eta_s.$$

Then for $r+1 \leq j \leq s$, we take $\mathbf{z}_j$ to be the unit row vector having an 1 in the η_j-th position and zeros elsewhere. Thus the canonical form of Theorem 2.6 (with all the $C^{(k)}$ taken to be ultratriangular forms with a consistent set of column indices) may be extended artificially to the s-fold sum

$$Q_\Lambda(f) = \frac{1}{d_1 d_2 \cdots d_s} \sum_{j_1=0}^{d_1-1} \sum_{j_2=0}^{d_2-1} \cdots \sum_{j_s=0}^{d_s-1} f\left(\left\{\sum_{i=1}^{s} j_i \frac{\mathbf{z}_i}{d_i}\right\}\right). \tag{2.11}$$

We then have the following definition.

Definition 2.8 *If the column indices for the ultratriangular forms of the Sylow p_k-components are consistent, then a standard $D - Z$ form is an s-cycle form in which*

(a) *Z is cpuut with column indices $\eta_1, \eta_2, \ldots, \eta_s$,*

(b) *$0 \leq z_{k,\eta_m} < d_k/d_m$, $1 \leq k < m \leq s$.*

It follows from Lemma 2.7 and the padding procedure described above that the $s \times s$ matrix Z can be assumed to be cpuut. If it is not already in standard form, then it can be transformed into standard form by using a sequence of transformations

$$\mathbf{z}'_k = \mathbf{z}_k - \left\lfloor \frac{z_{k,\eta_m} d_m}{d_k} \right\rfloor \frac{d_k}{d_m} \mathbf{z}_m, \quad k < m, \tag{2.12}$$

where $\lfloor a \rfloor$ denotes the largest integer less than or equal to a. Theorem 2.1(c) shows that such a transformation leaves the lattice rule Q_Λ unchanged. The transformation (2.12) affects only $\mathbf{z}_k$, the k-th row of Z. Moreover, since $\mathbf{z}_m$ has zeros in positions $\eta_1, \eta_2, \ldots, \eta_{m-1}$, the above transformation leaves the corresponding components of $\mathbf{z}_k$ unaltered, but generally alters the remaining components. In particular, since $z_{m,\eta_m} = 1$, we see that z_{k,η_m} is replaced by

$$z'_{k,\eta_m} = z_{k,\eta_m} - \left\lfloor \frac{z_{k,\eta_m} d_m}{d_k} \right\rfloor \frac{d_k}{d_m} = \left(\frac{z_{k,\eta_m} d_m}{d_k} - \left\lfloor \frac{z_{k,\eta_m} d_m}{d_k} \right\rfloor \right) \frac{d_k}{d_m},$$

which clearly satisfies Definition 2.8(b). Once z_{k,η_m} has been replaced by z'_{k,η_m}, then any further transformations of the form (2.12) must be ordered in such a way that the new component z'_{k,η_m} is not altered again. This property holds if we deal successively with $\mathbf{z}_1, \ldots, \mathbf{z}_{s-1}$, and in each vector $\mathbf{z}_k$ alter the components z_{k,η_j}, $k < j$, in order of increasing j.

Theorem 2.9 *The standard $D - Z$ form for lattice rules whose ultratriangular forms have a consistent set of column indices is unique.*

Proof. We shall use induction to prove that Z is unique. This proof is based on the proofs in [33, Lemma 5.3] and [16, Lemma 5.11].

Suppose Z and Z' are two alternative forms of a Z-matrix of rule Q_Λ, both in standard form. Both Z and Z' have the same column indices $\eta_1, \ldots, \eta_s$. Also, since both Z and Z' are cpuut, then they have the same η_1-th column (all components being zero except for the first element which is 1).

Let us suppose columns $\eta_1, \eta_2, \ldots, \eta_{m-1}$ of Z coincide with the corresponding columns of Z', but that for some k, $z_{k,\eta_m} \neq z'_{k,\eta_m}$. (Note that such a value of k must be less than m as both Z and Z' are cpuut.) We see from (2.11) that both $\mathbf{z}_k/d_k$ and $\mathbf{z}'_k/d_k$ belong to the integration lattice corresponding to Q_Λ. From the properties of a lattice, the difference

$$\frac{\mathbf{z}_k - \mathbf{z}'_k}{d_k},$$

also does. As such, it may be expressed as

$$\sum_{i=1}^{s} j_i \frac{\mathbf{z}_i}{d_i}. \tag{2.13}$$

Taking components $\eta_1, \eta_2, \ldots, \eta_{m-1}$ of (2.13) in turn, we find that $j_i = 0$ for $1 \leq i \leq m-1$. Consideration of the η_m-th component yields

$$\frac{z_{k,\eta_m} - z'_{k,\eta_m}}{d_k} = \sum_{i=m}^{s} j_i \frac{z_{i,\eta_m}}{d_i} = \frac{j_m}{d_m},$$

with the final equality following because $z_{i,\eta_m} = 0$ for all i satisfying $m+1 \leq i \leq s$. Thus

$$z_{k,\eta_m} - z'_{k,\eta_m} = j_m \frac{d_k}{d_m}. \tag{2.14}$$

Since z_{k,η_m} and z'_{k,η_m} are both in the interval $[0, d_k/d_m)$, it follows that (2.14) can be satisfied only if $j_m = 0$.

It follows from (2.14) that, contrary to the hypothesis, $z_{k,\eta_m} = z'_{k,\eta_m}$ for all k, and so column η_m of Z and Z' also coincide. Thus the hypothesis that columns $\eta_1, \eta_2, \ldots, \eta_{m-1}$ of Z and Z' coincide leads to the same being true of column η_m. It follows by induction that Z and Z' must be the same matrix. Thus we conclude that the Z-matrix in standard form must be unique. □

If the column indices happen to be $\eta_m = m$ for $1 \leq m \leq s$, so that the Z-matrix is unit upper triangular, then the corresponding lattice rule is projection-regular. In this case, Theorem 2.9 recovers the result found in [33]. If this is not the case, then postmultiplying Z by P (as mentioned earlier) would give a unit upper triangular matrix. Note that this result also shows that a lattice rule is projection-regular if its prime-power components are projection-regular.

By using the unique Z given in Definition 2.8, we may find the number of projection-regular rules having a given set of invariants. Hence, we have the following result.

Theorem 2.10 *The number of projection-regular lattice rules having invariants $d_1, d_2, \dots, d_s$ is given by*

$$d_1^{s-1} d_2^{s-3} \cdots d_{s-1}^{3-s} d_s^{1-s}.$$

Proof. The elements z_{km} for $1 \le k < m \le s$ in the Z-matrix of the standard form must satisfy $0 \le z_{km} < d_k/d_m$. Therefore, there are d_k/d_m possible choices for z_{km}. If we consider each column of the unique Z-matrix in turn, we find that the number of projection-regular lattice rules is given by

$$\left(\frac{d_1}{d_2}\right) \times \left(\frac{d_1}{d_3} \times \frac{d_2}{d_3}\right) \times \left(\frac{d_1}{d_4} \times \frac{d_2}{d_4} \times \frac{d_3}{d_4}\right) \times \cdots \times \left(\frac{d_1}{d_s} \times \frac{d_2}{d_s} \times \cdots \times \frac{d_{s-1}}{d_s}\right).$$

Simplifying this expression gives the desired result. This recovers the result found in [31]. □

2.5 Number of prime-power lattice rules having given column indices and invariants

As mentioned earlier, any prime-power rule can be written in a unique ultratriangular form in which the Z-matrix is cpuut with unique column indices. In this section we obtain a formula for the number of ultratriangular forms, and hence the number of prime-power lattice rules, with specified invariants $d_1 = p^{\alpha_1}, \dots, d_t = p^{\alpha_t}$ and column indices $\eta_1, \dots, \eta_t$. We shall denote this quantity by $\psi_s(p^{\alpha_1}, \dots, p^{\alpha_t}; \eta_1, \dots, \eta_t)$. In turn, this quantity will depend on the four quantities μ_i, $\hat{\mu}_i$, τ_i, and $\hat{\tau}_i$ for $1 \le i \le t$ which are defined below.

To aid the understanding of the definitions of these four quantities, we shall discuss them in the context of an example. This example is the $D - Z$ form of a prime-power rule in which $s = 6$, $p = 2$, Z is cpuut, and the column indices are given by $\eta_1 = 1$, $\eta_2 = 6$, $\eta_3 = 4$, $\eta_4 = 2$, and $\eta_5 = 5$. We take

$$D = \begin{bmatrix} 32 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & \mathsf{a} & \mathsf{a} & \mathsf{a} & \mathsf{a} & \mathsf{a} \\ 0 & \mathsf{a} & \mathsf{a} & \mathsf{a} & \mathsf{a} & 1 \\ 0 & \mathsf{a} & \mathsf{a} & 1 & \mathsf{a} & 0 \\ 0 & 1 & \mathsf{a} & 0 & \mathsf{a} & 0 \\ 0 & 0 & \mathsf{a} & 0 & 1 & 0 \end{bmatrix}, \qquad (2.15)$$

where the a represent integers.

For i satisfying $1 \le i \le t$, let μ_i be the number of column indices that are less than η_i and that have a subscript larger than i. Suppose these subscripts are $k_1^{(i)}, \ldots, k_{\mu_i}^{(i)}$, which for simplicity we shall write here as just $k_1, \ldots, k_{\mu_i}$. For the example above we have $\eta_1 = 1$ when $i = 1$. There are no column indices less than $\eta_1 = 1$ and hence $\mu_1 = 0$. When $i = 2$, $\eta_2 = 6$. The column indices η_1, η_3, η_4, and η_5 are all less than $\eta_2 = 6$. However, only the last three have a subscript larger than $i = 2$. Hence $\mu_2 = 3$ and the corresponding subscripts are $k_1 = 3, k_2 = 4$, and $k_3 = 5$. The other values of μ_i and k_j may be found in a similar manner and are given in Table 2.1 further on.

Note that if there exists a j satisfying $1 \le j \le \mu_i$ for which $p^{\alpha_i} = p^{\alpha_{k_j}}$, then there are no lattice rules having the given column indices because we would then have $p^{\alpha_i} = p^{\alpha_{k_j}}$ with $k_j > i$, but $\eta_{k_j} < \eta_i$ which, from Definition 2.3(e), is not permissible. Let us suppose that this is not the case. By definition, the subscripts $k_1, \ldots, k_{\mu_i}$ are all larger than i, so it follows from Definition 2.3(f) that

$$z_{i,\eta_{k_j}} \in [0, p^{\alpha_i}/p^{\alpha_{k_j}}).$$

However, these values are further restricted by Definition 2.3(d) because the μ_i column indices in question are all less than η_i. Of the $p^{\alpha_i - \alpha_{k_j}}$ possible values for $z_{i,\eta_{k_j}}$, only 1 in p of them will satisfy Definition 2.3(d). From this we conclude that the components of $\mathbf{z}_i$ in positions $\eta_{k_1}, \ldots, \eta_{k_{\mu_i}}$ may be chosen in

$$\prod_{j=1}^{\mu_i} p^{\alpha_i - \alpha_{k_j} - 1} \tag{2.16}$$

ways.

Now denote by $\hat{\mu}_i$ the number of column indices that are less than η_i and that have a subscript less than i. For $i = 1$ in the example above, $\eta_1 = 1$ and there are no column indices less than 1, so that $\hat{\mu}_1 = 0$. When $i = 2$, $\eta_2 = 6$ and though there are four column indices less than $\eta_2 = 6$, only one of them, namely $\eta_1 = 1$ has a subscript less than $i = 2$. Hence, $\hat{\mu}_2 = 1$. The remaining values of $\hat{\mu}_i$ are given in Table 2.1.

Because the Z-matrix is cpuut, the components of $\mathbf{z}_i$ have to be zero in the positions specified by these $\hat{\mu}_i$ column indices. Thus, so far, of the components of $\mathbf{z}_i$ in positions $1, \ldots, \eta_i - 1$, we have accounted for $\mu_i + \hat{\mu}_i$ of them. Each of the remaining $\eta_i - 1 - \mu_i - \hat{\mu}_i$ components have to belong to $[0, p^{\alpha_i})$, but also satisfy Definition 2.3(d) from which we conclude that the number of possibilities is

$$\left[p^{\alpha_i - 1}\right]^{\eta_i - 1 - \mu_i - \hat{\mu}_i}. \tag{2.17}$$

Similarly, let τ_i be the number of column indices that are larger than η_i and that have a subscript larger than i. The corresponding subscripts are denoted by $\ell_1^{(i)}, \ldots, \ell_{\tau_i}^{(i)}$, which we write here as simply $\ell_1, \ldots, \ell_{\tau_i}$. For $i = 1$ in the example above, $\eta_1 = 1$ and all the column indices η_2, η_3, η_4, and η_5 are larger than $\eta_1 = 1$. Moreover, their subscripts are all larger than $i = 1$. Therefore, $\tau_1 = 4$ and the corresponding subscripts are given by $\ell_1 = 2, \ell_2 = 3$, $\ell_3 = 4$, and $\ell_4 = 5$. When $i = 2$ there are no column indices larger than $\eta_2 = 6$ so that $\tau_2 = 0$. Table 2.1 contains the other values of τ_i and ℓ_j.

Definition 2.3(f) shows that

$$z_{i,\eta_{\ell_j}} \in [0, p^{\alpha_i}/p^{\alpha_{\ell_j}}).$$

Since these τ_i column indices are larger than η_i, the restriction of Definition 2.3(d) does not apply and we conclude that the number of ways of choosing the components of $\mathbf{z}_i$ in positions $\eta_{\ell_1}, \ldots, \eta_{\ell_{\tau_i}}$ is

$$\prod_{j=1}^{\tau_i} p^{\alpha_i - \alpha_{\ell_j}}. \tag{2.18}$$

Finally, let us denote by $\hat{\tau}_i$ the number of column indices that are larger than η_i and that have a subscript less than i. It follows from the definitions of $\mu_i, \hat{\mu}_i$, and τ_i that $\mu_i + \hat{\mu}_i + \tau_i + \hat{\tau}_i = t - 1$. Hence, we have

$$\hat{\tau}_i = t - 1 - \mu_i - \hat{\mu}_i - \tau_i.$$

Because the Z-matrix is cpuut, the components of $\mathbf{z}_i$ have to be zero in the positions specified by these $\hat{\tau}_i$ column indices. Thus, so far, of the components of $\mathbf{z}_i$ in positions $\eta_i + 1, \ldots, s$, we have accounted for $\tau_i + \hat{\tau}_i$ of them. Each of the remaining $s - \eta_i - \tau_i - \hat{\tau}_i$ components have to belong to $[0, p^{\alpha_i})$, from which we conclude that the number of possibilities is

$$\left[p^{\alpha_i}\right]^{s - \eta_i - \tau_i - \hat{\tau}_i}. \tag{2.19}$$

This discussion and equations (2.16)–(2.19) lead to the following result.

Theorem 2.11 *For $1 \le i \le t$, let μ_i be the number of column indices that are less than η_i and that have a subscript larger than i. Suppose that the subscripts of these column indices are $k_1^{(i)}, \ldots, k_{\mu_i}^{(i)}$. Now denote by $\hat{\mu}_i$ the number of column indices that are less than η_i and whose subscript is less than i. Similarly, let τ_i be the number of column indices larger than η_i and that have a subscript larger than i. The corresponding subscripts are denoted by $\ell_1^{(i)}, \ldots, \ell_{\tau_i}^{(i)}$. Finally, let $\hat{\tau}_i = t - 1 - \mu_i - \hat{\mu}_i - \tau_i$. Then define $\kappa_i := 0$ if $\alpha_i = \alpha_{k_j^{(i)}}$ for any j satisfying $1 \le j \le \mu_i$; otherwise define*

$$\kappa_i := \left[\prod_{j=1}^{\mu_i} p^{\alpha_i - \alpha_{k_j^{(i)}} - 1}\right] \times \left[p^{\alpha_i - 1}\right]^{\eta_i - 1 - \mu_i - \hat{\mu}_i} \times \left[\prod_{j=1}^{\tau_i} p^{\alpha_i - \alpha_{\ell_j^{(i)}}}\right] \times \left[p^{\alpha_i}\right]^{s - \eta_i - \tau_i - \hat{\tau}_i},$$

where empty products are taken to be 1, that is, when μ_i and/or τ_i are zero. The number of prime-power lattice rules with given invariants $p^{\alpha_1}, \ldots, p^{\alpha_t}$ and column indices $\eta_1, \ldots, \eta_t$ is

$$\psi_s(p^{\alpha_1}, \ldots, p^{\alpha_t}; \eta_1, \ldots, \eta_t) = \prod_{i=1}^{t} \kappa_i.$$

Table 2.1: The values of the parameters.

i	η_i	α_i	μ_i	$\hat{\mu}_i$	τ_i	$\hat{\tau}_i$	$k_1^{(i)}$	$k_2^{(i)}$	$k_3^{(i)}$	$\ell_1^{(i)}$	$\ell_2^{(i)}$	$\ell_3^{(i)}$	$\ell_4^{(i)}$	κ_i
1	1	5	0	0	4	0	-	-	-	2	3	4	5	32768
2	6	4	3	1	0	0	3	4	5	-	-	-	-	64
3	4	3	1	1	1	1	4	-	-	5	-	-	-	16
4	2	2	0	1	1	2	-	-	-	5	-	-	-	8
5	5	1	0	3	0	1	-	-	-	-	-	-	-	1

For the $D-Z$ form given in (2.15), the full list of values for the various parameters are given in Table 2.1. The total number of prime-power lattice rules having $D = \mathrm{diag}\{32, 16, 8, 4, 2\}$ and column indices given by $1, 6, 4, 2, 5$ is

$$\prod_{i=1}^{5} \kappa_i = 32768 \times 64 \times 16 \times 8 \times 1 = 268,435,456.$$

As another simple example, we consider the case of projection-regular rules which we recall are rules for which $\eta_i = i$. Such rules have the $D - Z$ form given by

$$D = \begin{bmatrix} p^{\alpha_1} & 0 & 0 & 0 & & 0 \\ 0 & p^{\alpha_2} & 0 & 0 & & 0 \\ 0 & 0 & p^{\alpha_3} & 0 & & 0 \\ 0 & 0 & 0 & p^{\alpha_4} & \cdots & 0 \\ & & & & & \\ 0 & 0 & 0 & 0 & & p^{\alpha_t} \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & \mathsf{a} & \mathsf{a} & \mathsf{a} & \cdots & \mathsf{a} \\ 0 & 1 & \mathsf{a} & \mathsf{a} & \cdots & \mathsf{a} \\ 0 & 0 & 1 & \mathsf{a} & \cdots & \mathsf{a} \\ 0 & 0 & 0 & 1 & \cdots & \mathsf{a} \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

It is not difficult to see from the $D - Z$ form that $\mu_i = 0$, $\hat{\mu}_i = i - 1$, $\tau_i = t - i$, $\ell_j^{(i)} = i + j$, and $\hat{\tau}_i = 0$. Using these values, we find that

$$\prod_{j=1}^{\mu_i} p^{\alpha_i - \alpha_{k_j^{(i)}} - 1} = \left[p^{\alpha_i - 1}\right]^{\eta_i - 1 - \mu_i - \hat{\mu}_i} = 1$$

and

$$\prod_{j=1}^{\tau_i} p^{\alpha_i - \alpha_{\ell_j^{(i)}}} = \prod_{j=1}^{t-i} p^{\alpha_i - \alpha_{i+j}}, \quad [p^{\alpha_i}]^{s - \eta_i - \tau_i - \hat{\tau}_i} = [p^{\alpha_i}]^{s-t}.$$

Hence, the total number of projection-regular prime-power lattice rules having invariants $p^{\alpha_1}, \ldots, p^{\alpha_t}$ is

$$\prod_{i=1}^{t} \kappa_i = \prod_{i=1}^{t} \left[\left(\prod_{j=1}^{t-i} p^{\alpha_i - \alpha_{i+j}} \right) [p^{\alpha_i}]^{s-t} \right].$$

Upon expanding this last expression out and collecting the p^{α_i} terms together, we find that this expression is equivalent to

$$\prod_{i=1}^{t} (p^{\alpha_i})^{s-2i+1} = (p^{\alpha_1})^{s-1}(p^{\alpha_2})^{s-3}(p^{\alpha_3})^{s-5} \ldots (p^{\alpha_{t-1}})^{s-2t+3}(p^{\alpha_t})^{s-2t+1},$$

which recovers the result found in Theorem 2.10, in the case when $d_i = p^{\alpha_i}$ for $1 \leq i \leq t$. We remark that if $t = s$, this result is equivalent to that given in Theorem 2.10. This is also the case if $t < s$ since $d_{t+1} = d_{t+2} = \cdots = d_s = 1$.

Chapter 3

A lower triangular Hermite normal form for projection-regular lattice rules

3.1 Chapter summary

The structure of lattice rules has been studied using two different approaches. One of them is based on the generator matrices A and B of the integration lattice Λ and its dual $\Lambda^{\perp}$, respectively and the other approach is based on the representation of lattice rules in t-cycle $D-Z$ forms. This latter approach was previously used to find unique forms for prime-power and projection-regular lattice rules. It was also used in Chapter 2 to obtain a unique form for a special class of lattice rules whose ultratriangular components have a consistent set of column indices. It is known that by using row operations any integer matrix may be expressed uniquely in a so-called Hermite normal form (see [30]). This unique form may either be upper triangular or lower triangular. The former approach based on the generator matrix of the dual lattice has previously made the assumption that it is upper triangular. However, since the unique Z for the special case of projection-regular rules is upper triangular, the corresponding B turns out to be lower triangular. This suggests that the lower triangular Hermite normal form might be an appropriate form to study. In this chapter we consider such representations for projection-regular rules. We shall obtain a unique representation for the generator matrix B of the dual lattice for such rules. This is done by making use of their unique $D-Z$ form. The results obtained give conditions on the generator matrix which allow projection-regular rules to be easily recognized. In Section 3.2 we give results from Chapter 2 relating to the unique $D-Z$ form for projection-regular rules. In Section 3.3 results concerning the upper triangular lattice form are given and in the final section, Section 3.4, we define a unique lower triangular form for the generator matrix of the dual lattice (which is a special case of the lower triangular Hermite normal form) in the case of projection-regular rules.

3.2 Unique $D-Z$ form for projection-regular lattice rules

Projection-regular rules, as mentioned earlier, are special classes of lattice rules in which all the principal projections have the maximum possible order.

Example 3.1 *The three-dimensional lattice rule given by*

$$\frac{1}{12}\sum_{i_1=0}^{5}\sum_{i_2=0}^{1} f\left(\left\{i_1\frac{(1,2,1)}{6}+i_2\frac{(1,1,1)}{2}\right\}\right),$$

is a projection-regular rule. The rank of this rule is 2 *and it has the invariants* $d_1=6, d_2=2, d_3=1$. *The two-dimensional principal projection of this rule given by*

$$\frac{1}{12}\sum_{i_1=0}^{5}\sum_{i_2=0}^{1} f\left(\left\{i_1\frac{(1,2)}{6}+i_2\frac{(1,1)}{2}\right\}\right),$$

has invariants $d_1=6, d_2=2$. *Similarly one may show that the one-dimensional principal projection has the sole invariant* 6.

The rest of this section shall be devoted to defining a unique $D-Z$ form for projection-regular rules. The results given here follow from Chapter 2 and were first obtained in [33]. Recall that every lattice rule may be expressed in a canonical $D - Z$ form

$$Q_\Lambda(f) = \frac{1}{d_1 d_2 \cdots d_r} \sum_{i_1=0}^{d_1-1} \sum_{i_2=0}^{d_2-1} \cdots \sum_{i_r=0}^{d_r-1} f\left(\left\{i_1 \frac{\mathbf{z}_1}{d_1} + i_2 \frac{\mathbf{z}_2}{d_2} + \cdots + i_r \frac{\mathbf{z}_r}{d_r}\right\}\right),$$

where r and $d_1, d_2, \ldots, d_r$ are uniquely determined positive integers known as the rank and invariants respectively. This form may be extended artificially (as done in (2.11)) to the s-fold sum

$$Q_\Lambda(f) = \frac{1}{d_1 d_2 \cdots d_s} \sum_{i_1=0}^{d_1-1} \sum_{i_2=0}^{d_2-1} \cdots \sum_{i_s=0}^{d_s-1} f\left(\left\{i_1 \frac{\mathbf{z}_1}{d_1} + i_2 \frac{\mathbf{z}_2}{d_2} + \cdots + i_s \frac{\mathbf{z}_s}{d_s}\right\}\right), \tag{3.1}$$

where $d_{r+1} = \cdots = d_s = 1$ and $\mathbf{z}_{r+1}, \ldots, \mathbf{z}_s$ are arbitrary integer vectors. Although the matrix D is uniquely determined in the extended form (3.1), the vectors $\mathbf{z}_i$, and hence the $s \times s$ matrix Z given by

$$Z = \begin{bmatrix} \mathbf{z}_1 \\ \\ \mathbf{z}_s \end{bmatrix},$$

with z_{ij} denoting the j-th component of $\mathbf{z}_i$, is not. However, for projection-regular rules this matrix may be made unique. This unique form is given in the following theorem and is a consequence of Definition 2.8 and Theorem 2.9 in which we take $\eta_i = i$ for $1 \le i \le s$.

Theorem 3.1 *Suppose we have a canonical s-cycle $D - Z$ form for a projection-regular rule. Moreover, suppose the matrix Z has the following properties*

(a) $z_{ij} = 0, \quad 1 \le j < i \le s,$

(b) $z_{ii} = 1, \quad 1 \le i \le s,$

(c) $0 \le z_{ij} < \frac{d_i}{d_j}, \quad 1 \le i < j \le s.$

Then such a Z is unique.

Example 3.2 *The projection-regular rule given in Example 3.1 has the $D' - Z'$ representation*

$$D' = \begin{bmatrix} 6 & 0 \\ 0 & 2 \end{bmatrix}, \quad Z' = \begin{bmatrix} 1 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

By using the procedure given in Chapter 2, one may verify that the unique $D - Z$ form for this rule is given by

$$D = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

3.3 The upper triangular lattice form

An $s \times s$ generator matrix A of the integration lattice Λ contains a generator $\mathbf{a}_i$ in its i-th row. Since any given Λ may have many such generator matrices, the matrix A is not unique. In fact, one may carry out elementary row operations on A (using integer coefficients) without changing the lattice Λ; that is, we may premultiply A by a unimodular matrix (a square matrix having a determinant -1 or 1) without changing the lattice.

The integer matrix B of the dual lattice $\Lambda^{\perp}$ is related to the matrix A by the matrix equation, $B = (A^T)^{-1}$ (see [20]). Given one of the matrices A or B, we may obtain the other by using this relation. In terms of these matrices, the order of the lattice rule Q_Λ is given by

$$\nu(Q_\Lambda) = |\det A|^{-1} = |\det B|.$$

Like the matrix A, the matrix B is not unique since a lattice generated by B may also be generated by $B' = TB$, where T is any unimodular matrix. However, successive row operations may be carried out to put B in an upper triangular lattice form, defined below. An algorithm for doing this may be found in [19].

Definition 3.2 *An $s \times s$ integer matrix B is in upper triangular lattice form if and only if*

(a) $b_{ii} \geq 1, \quad 1 \leq i \leq s,$

(b) $b_{ij} = 0, \quad 1 \leq j < i \leq s,$

(c) $0 \leq b_{ij} < b_{jj}, \quad$ otherwise.

Example 3.3 *A matrix B' and its upper triangular lattice form B are given by*

$$B' = \begin{bmatrix} 1 & 3 & 4 \\ 4 & 2 & 6 \\ 0 & 2 & 4 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 2 & 4 \\ 0 & 0 & 10 \end{bmatrix}.$$

The above definition then leads us to the following result found in [19].

Theorem 3.3 *Every dual lattice $\Lambda^\perp$ has a unique generator matrix B in upper triangular lattice form.*

This unique form is essentially the Hermite normal form and it has previously been used to derive many useful results in the field of lattice rules (see for example, [20], [21] and [22]).

In the section that follows, we will consider the lower triangular lattice form of the matrix B for lattice rules. This form will then be used to define a unique lower triangular representation of this matrix B for the special case of projection-regular rules.

3.4 A unique lower triangular form for projection-regular rules

In order to obtain a unique lower triangular representation for the matrix B of projection-regular rules, we shall first define the lower triangular lattice form for the matrix B of any lattice rule. This is defined in the following way.

Definition 3.4 *An $s \times s$ matrix B is in lower triangular lattice form if and only if*

(a) $b_{ii} \geq 1, \quad 1 \leq i \leq s,$

(b) $b_{ij} = 0, \quad 1 \leq i < j \leq s,$

(c) $0 \leq b_{ij} < b_{jj}, \quad$ otherwise.

We may use row operations to transform any given integer matrix into a lower triangular form. After this is done or during the process of doing this, it is straightforward to arrange the subdiagonal elements such that they satisfy condition (c) of the above definition. We then have the following analogue of Theorem 3.3.

Theorem 3.5 *Every dual lattice $\Lambda^{\perp}$ has a unique generator matrix B in lower triangular lattice form.*

Proof. The result follows from [30, Theorem 4.2]. □

For projection-regular rules, the unique Z-matrix given in Theorem 3.1 is unimodular since it is upper triangular with all the elements in the diagonal being 1. In order to derive a corresponding unique lower triangular form for the matrix B from this unique $D - Z$ form, we require the following result from [18].

Theorem 3.6 *Suppose that Q_Λ is given in an s-cycle $D - Z$ form with a Z-matrix that is unimodular. Then this $D - Z$ representation is non-repetitive and the matrix A defined by $A = D^{-1}Z$ is a generator matrix of the lattice Λ.*

Hence, we may use the unique Z, given in Theorem 3.1, to obtain the generator matrix $A = D^{-1}Z$ for projection-regular rules. For such rules having the rank r and the unique $D - Z$ form given by

$$D = \begin{bmatrix} d_1 & 0 & 0 & \cdots & 0 \\ & & & & \vdots \\ 0 & d_r & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & \cdots & z_{1,r} & z_{1,r+1} & z_{1,s} \\ \vdots & & & & \\ 0 & \cdots & 1 & z_{r,r+1} & z_{r,s} \\ 0 & \cdots & 0 & 1 & 0 \\ \vdots & & & & \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix}, \tag{3.2}$$

the generator matrix A has the form

$$A = \begin{bmatrix} \frac{1}{d_1} & \cdots & \frac{z_{1,r}}{d_1} & \frac{z_{1,r+1}}{d_1} & \cdots & \frac{z_{1,s}}{d_1} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & & \frac{1}{d_r} & \frac{z_{r,r+1}}{d_r} & \cdots & \frac{z_{r,s}}{d_r} \\ 0 & & 0 & 1 & & 0 \\ & & & & & \\ 0 & & 0 & 0 & & 1 \end{bmatrix}.$$

From this matrix, we may obtain the generator matrix $B = (A^T)^{-1}$. Alternatively, we may obtain B directly from the $D - Z$ form by using $B = D(Z^T)^{-1}$. Thus we have the following result.

Theorem 3.7 *For a rank-r projection-regular lattice rule having the unique $D - Z$ form given in* (3.2), *the matrix $B = D(Z^T)^{-1}$ is given by*

$$b_{ij} = \begin{cases} 0, & j > i \quad or \quad r < j < i, \\ \Phi_i, & j = i \quad and \quad 1 \leq i \leq s, \\ \Phi_i \sum\limits_{\mathbf{K} \in S_{ij}} z_{jk_1} z_{k_1 k_2}, \cdots z_{k_\theta i} \times \operatorname{sign}(\mathbf{K}), & j < i \quad and \quad j \leq r, \end{cases} \tag{3.3}$$

where $\Phi_i = d_i$ for $1 \leq i \leq r$ and $\Phi_i = 1$ otherwise. Moreover, the elements of the set S_{ij} are generalized integers $\mathbf{K} = (k_1, k_2, \ldots, k_\theta)$ such that

$$j < k_1 < k_2 < \cdots < k_\theta < i.$$

The set S_{ij} is empty when $i = j + 1$ and it may contain at most 2^{i-j-1} elements (because $z_{\ell m} = 0$ for $r < \ell < m$, some of the elements vanish). Associated with each $\mathbf{K}$ is $\operatorname{sign}(\mathbf{K}) = (-1)^{\theta+1}$ which takes the value 1 when the number of integers is odd and the value -1 when the number of integers is even including zero.

Proof. This result follows from [19, p. 15]. □

To give a better understanding of the form (3.3) for the matrix B, we now give two examples.

Example 3.4 *For a six-dimensional projection-regular rule with rank* 2*, the matrix* $B = D(Z^T)^{-1}$ *is given by*

$$B = \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 & 0 \\ -z_{12}d_2 & d_2 & 0 & 0 & 0 & 0 \\ z_{12}z_{23} - z_{13} & -z_{23} & 1 & 0 & 0 & 0 \\ z_{12}z_{24} - z_{14} & -z_{24} & 0 & 1 & 0 & 0 \\ z_{12}z_{25} - z_{15} & -z_{25} & 0 & 0 & 1 & 0 \\ z_{12}z_{26} - z_{16} & -z_{26} & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Example 3.5 *For a six-dimensional rank-*3 *projection-regular lattice rule, the matrix* $B = D(Z^T)^{-1}$ *is given by*

$$B = \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 & 0 \\ -z_{12}d_2 & d_2 & 0 & 0 & 0 & 0 \\ (z_{12}z_{23} - z_{13})d_3 & -z_{23}d_3 & d_3 & 0 & 0 & 0 \\ -z_{12}z_{23}z_{34} + z_{12}z_{24} + z_{13}z_{34} - z_{14} & z_{23}z_{34} - z_{24} & -z_{34} & 1 & 0 & 0 \\ -z_{12}z_{23}z_{35} + z_{12}z_{25} + z_{13}z_{35} - z_{15} & z_{23}z_{35} - z_{25} & -z_{35} & 0 & 1 & 0 \\ -z_{12}z_{23}z_{36} + z_{12}z_{26} + z_{13}z_{36} - z_{16} & z_{23}z_{36} - z_{26} & -z_{36} & 0 & 0 & 1 \end{bmatrix}.$$

Notice that the matrix B, given in (3.3), is lower triangular. This justifies our decision to consider lower triangular representations for projection-regular rules. Once we have the matrix B in this form, we may carry out a series of row operations on it such that it becomes a special case of the lower triangular lattice form given in Definition 3.4. We then have the following result.

Theorem 3.8 *Let a rank-r projection-regular lattice rule be given in the unique* $D - Z$ *form, as defined in Theorem 3.1. Then the matrix* B *given by* $B = D(Z^T)^{-1}$ *may be expressed uniquely in lower triangular lattice form with elements satisfying*

(a) $b_{ii} = d_i, \quad 1 \leq i \leq s,$

(b) $b_{ij} = 0, \quad 1 \leq i < j \leq s,$

(c) $0 \leq b_{ij} < b_{jj}, \quad 1 \leq j < i \leq s,$

(d) $b_{ij}/b_{ii} \in \mathbb{Z}$*; that is,* b_{ij} *has a factor* $b_{ii} = d_i, \quad j < i \leq r.$

Proof. In order to transform the matrix B given in (3.3) into this lower triangular lattice form, we may carry out row operations of the form,

$$\mathbf{b}_i' = \mathbf{b}_i + \lambda \mathbf{b}_j, \quad \text{where} \quad \lambda \in \mathbb{Z}, \quad i \neq j. \tag{3.4}$$

The matrix B given in (3.3) is already in a lower triangular form with d_i's on the main diagonal. Thus, we only need to make the entries b_{ij} lying below the main diagonal nonnegative and less than b_{jj}. This may be done by using the row operation (3.4) with $\lambda = -\left\lfloor \frac{b_{ij}}{b_{jj}} \right\rfloor$. In particular, the j-th component of $\mathbf{b}_i'$ is given by

$$b_{ij}' = b_{ij} - \left\lfloor \frac{b_{ij}}{b_{jj}} \right\rfloor b_{jj} = \left(\frac{b_{ij}}{b_{jj}} - \left\lfloor \frac{b_{ij}}{b_{jj}} \right\rfloor \right) b_{jj},$$

which clearly satisfies $0 \leq b_{ij}' < b_{jj}$. These row operations must be ordered in such a way that once b_{ij} is changed, it is not altered again. This is achieved if the row operations are carried out in the following order. In (3.4), for every value of i going from s down to $r+1$ we take j from r down to 1. Then all the elements below the r-th row will satisfy the conditions of the above theorem.

The rest of the entries b_{ij} for $j < i \leq r$ must also be less than b_{jj}. For these entries we perform the above row operation by taking for every value of i from r down to 2, the values of j from $i-1$ down to 1. We need to verify that the non-trivial factors d_i are preserved in these entries. To do this, we note that the entries b_{ij} and d_j both have the factor d_i for $j < i \leq r$ (this follows from Theorem 3.7 and the fact that $d_{i+1} \mid d_i$ for $1 \leq i < r$, respectively); that is,

$$b_{ij} = \beta_1 d_i, \quad d_j = \beta_2 d_i,$$

where $\beta_1, \beta_2 \in \mathbb{Z}$. It then follows that

$$b_{ij}' = b_{ij} - \left\lfloor \frac{b_{ij}}{b_{jj}} \right\rfloor b_{jj} = d_i \left(\beta_1 - \left\lfloor \frac{\beta_1}{\beta_2} \right\rfloor \beta_2 \right).$$

Hence, the factors d_i are preserved in entries b_{ij} for $j < i \leq r$. □

We remark that the unique B, given in Theorem 3.8, may be used to obtain the number of projection-regular rules having a given set of invariants. This may be done by first noting that the entries b_{ij} for $j < i \leq r$ have a factor d_i. Moreover, entries b_{ij} in the j-th column of B must satisfy $b_{ij} < d_j$. Hence the total number of choices for b_{ij} when $j < i \le r$ is d_j/d_i. The rest of the entries b_{ij} below the diagonal must be less that d_j. By considering each of the columns of this unique B in turn, we see that the total number of possibilities correspond to the number of projection-regular lattice rules, as given in Theorem 2.10.

Example 3.6 *The seven-dimensional rank-4 projection-regular lattice rule with the unique $D - Z$ form given by*

$$D = \begin{bmatrix} 216 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 54 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 27 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 3 & 7 & 23 & 174 & 201 & 89 \\ 0 & 1 & 1 & 5 & 43 & 51 & 13 \\ 0 & 0 & 1 & 2 & 19 & 23 & 25 \\ 0 & 0 & 0 & 1 & 8 & 5 & 7 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

has the matrix $B = D(Z^T)^{-1}$ given by

$$B = \begin{bmatrix} 216 & 0 & 0 & 0 & 0 & 0 & 0 \\ -162 & 54 & 0 & 0 & 0 & 0 & 0 \\ -108 & -27 & 27 & 0 & 0 & 0 & 0 \\ 0 & -27 & -18 & 9 & 0 & 0 & 0 \\ 31 & 0 & -3 & -8 & 1 & 0 & 0 \\ 44 & -13 & -13 & -5 & 0 & 1 & 0 \\ 50 & 33 & -11 & -7 & 0 & 0 & 1 \end{bmatrix}.$$

After carrying out the row operations on this matrix, as described above, we get the *lower triangular lattice form of B given by*

$$B = \begin{bmatrix} 216 & 0 & 0 & 0 & 0 & 0 & 0 \\ 54 & 54 & 0 & 0 & 0 & 0 & 0 \\ 162 & 27 & 27 & 0 & 0 & 0 & 0 \\ 162 & 0 & 9 & 9 & 0 & 0 & 0 \\ 193 & 0 & 6 & 1 & 1 & 0 & 0 \\ 152 & 14 & 23 & 4 & 0 & 1 & 0 \\ 104 & 6 & 25 & 2 & 0 & 0 & 1 \end{bmatrix}.$$

We remark that if we have a matrix B in the form defined by (a)–(d) of Theorem 3.8, then it always represents a projection-regular rule with the rank equal to the number of non-unit entries in the main diagonal.

Chapter 4

The L_2 discrepancy for quasi-Monte Carlo rules

4.1 Chapter summary

In the theory of quasi-Monte Carlo rules, we have error bounds of the form

$$|I(f) - Q(f)| \leq D(Q)V(f), \tag{4.1}$$

where $V(f)$ is a measure of variation of the integrand and the quantity $D(Q)$ measures the non-uniformity of the point set. In this thesis, we shall take the measure of non-uniformity to be the L_2 (star) discrepancy. Hence, we present in this chapter, two methods of obtaining an expression for this quantity. The first method is by making use of local discrepancy and the second one is by using reproducing kernel Hilbert spaces. These are described in sections 4.2 and 4.3, respectively. In Section 4.4, we obtain the expected value of the squared discrepancy for Monte Carlo rules and in the final section, Section 4.5, we give a periodic version of the bound (4.1) and hence give the appropriate L_2 discrepancy.

4.2 The Koksma-Hlawka inequality

In the approximation of multidimensional integrals over the s-dimensional unit cube, the performance of quasi-Monte Carlo equal-weight rules of the form (1.2) depends on the distribution of the points $\mathbf{t}_0, \ldots, \mathbf{t}_{n-1}$ over the unit cube $[0,1]^s$. In general, if these points are evenly distributed over the unit cube, then they tend to provide good approximations to the integral (1.1) (as mentioned in [12]). Thus, in order to study the error in quasi-Monte Carlo rules, we need a quantity to measure how far a set of points is from the ideal uniform distribution. One such quantity is the classical L_2 discrepancy which is defined in terms of the local discrepancy

$$g(\mathbf{t}) = \frac{\psi([0,t_1) \times \cdots \times [0,t_s))}{n} - t_1 \cdots t_s, \tag{4.2}$$

where $\psi([0,t_1) \times \cdots \times [0,t_s))$ is the number of points of the original rule Q (see (1.2)) that lie in the region $[0,t_1) \times \cdots \times [0,t_s)$. The classical L_2 discrepancy is then given by

$$\hat{D}(Q) = \left(\int_{[0,1]^s} g^2(\mathbf{t})\, \mathrm{d}\mathbf{t} \right)^{1/2}$$

A simple expression (as found in [36]) for this quantity is given by

$$\hat{D}^2(Q) = \left(\frac{1}{3}\right)^s - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{1}{2} - \frac{t_{i,j}^2}{2} \right) + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{s} \left[1 - \max(t_{i,j}, t_{k,j})\right].$$

where $\mathbf{t}_i = (t_{i,1}, t_{i,2}, \ldots, t_{i,s})$. It has been proved by Woźniakowski [37] that this discrepancy is the average-case error with respect to the Wiener sheet measure. In this thesis, we shall use $D(Q)$, the L_2 discrepancy which will be defined below.

For a nonempty subset $\mathbf{u}$ of $S = \{1, 2, \ldots, s\}$ let the cardinality be given by $|\mathbf{u}|$ and for $\mathbf{t} \in [0,1]^s$ let $\mathbf{t_u}$ denote the vector from $[0,1]^{|\mathbf{u}|}$ containing the components of $\mathbf{t}$ whose indices belong to $\mathbf{u}$. Also let $(\mathbf{t_u}, \mathbf{1})$ be the vector obtained from $\mathbf{t}$ after the components with indices not in $\mathbf{u}$ are replaced by 1. It then follows from [38] that for integrands f, with bounded variation $V(f)$ on $[0,1]^s$ in the sense of Hardy and Krause, the error bound for quasi-Monte Carlo rules is given by (4.1), where the L_2 discrepancy is given by

$$D(Q) = \left(\sum_{\emptyset \neq \mathbf{u} \subseteq S} \int_{[0,1]^{|\mathbf{u}|}} g^2(\mathbf{t_u}, \mathbf{1})\, \mathrm{d}\mathbf{t_u} \right)^{1/2} \tag{4.3}$$

and $V(f)$ is a measure of the variation of f given by

$$V(f) = \left(\sum_{\emptyset \neq \mathbf{u} \subseteq S} \int_{[0,1]^{|\mathbf{u}|}} \left| \frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{t_u}} f(\mathbf{t_u}, \mathbf{1}) \right|^2 \mathrm{d}\mathbf{t_u} \right)^{1/2} \tag{4.4}$$

The inequality (4.1) together with (4.3) and (4.4) is known as the L_2 version of the Koksma-Hlawka inequality and it relates the error to the variation of the integrand. We note that this L_2 discrepancy incorporates the classical L_2 discrepancy of the projections of the points $\mathbf{t}_0, \ldots, \mathbf{t}_{n-1}$ onto lower-dimensional faces of the unit cube $[0,1]^s$. In this section and the next we shall find an expression for $D^2(Q)$ using two methods. Here, we make use of (4.3) to obtain an expression.

If $\mathbf{t} = (t_1, t_2, \ldots, t_s)$ and $\mathbf{t}_i = (t_{i,1}, t_{i,2}, \ldots, t_{i,s})$, then the local discrepancy (4.2) at the point $(\mathbf{t}_\mathbf{u}, \mathbf{1})$ may be written as

$$g(\mathbf{t}_\mathbf{u}, \mathbf{1}) = \frac{1}{n}\sum_{i=0}^{n-1}\prod_{j\in\mathbf{u}} I_{t_{i,j}<t_j} - \prod_{j\in\mathbf{u}} t_j, \tag{4.5}$$

where $I_{t_{i,j}<t_j}$ is the indicator function

$$I_{t_{i,j}<t_j} = \begin{cases} 1, & t_{i,j} < t_j, \\ 0, & t_{i,j} \geq t_j. \end{cases}$$

The square of $g(\mathbf{t}_\mathbf{u}, \mathbf{1})$ may be written as

$$g^2(\mathbf{t}_\mathbf{u}, \mathbf{1}) = \prod_{j\in\mathbf{u}} t_j^2 - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j\in\mathbf{u}} t_j I_{t_{i,j}<t_j} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j\in\mathbf{u}} I_{t_{i,j}<t_j} I_{t_{k,j}<t_j}.$$

Noting that

$$\int_0^1 t_j^2 \,\mathrm{d}t_j = \frac{1}{3}, \qquad \int_0^1 t_j I_{t_{i,j}<t_j} \,\mathrm{d}t_j = \int_{t_{i,j}}^1 t_j \,\mathrm{d}t_j = \frac{1}{2}\left(1 - t_{i,j}^2\right)$$

and

$$\int_0^1 I_{t_{i,j}<t_j} I_{t_{k,j}<t_j} \,\mathrm{d}t_j = \int_{\max(t_{i,j}, t_{k,j})}^1 1 \,\mathrm{d}t_j = 1 - \max(t_{i,j}, t_{k,j}),$$

the expression for the squared L_2 discrepancy is given by

$$\begin{aligned} D^2(Q) &= \sum_{\emptyset\neq\mathbf{u}\subseteq S} \int_{[0,1]^{|\mathbf{u}|}} g^2(\mathbf{t}_\mathbf{u}, \mathbf{1}) \,\mathrm{d}\mathbf{t}_\mathbf{u} \\ &= \sum_{\emptyset\neq\mathbf{u}\subseteq S} \left[\left(\frac{1}{3}\right)^{|\mathbf{u}|} - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j\in\mathbf{u}}\frac{1}{2}\left(1 - t_{i,j}^2\right) + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j\in\mathbf{u}}\left[1 - \max(t_{i,j}, t_{k,j})\right]\right]. \end{aligned} \tag{4.6}$$

We remark that this expression for the L_2 discrepancy is not very useful for computational purposes. It involves a sum over all nonempty subsets of the set S. We note that the number of subsets of this set having $|\mathbf{u}|$ elements is $\binom{s}{|\mathbf{u}|}$ and the product under the double summation has $|\mathbf{u}|$ terms. Moreover, we note from equation 0.154 of Gradshteyn and Ryzhik [7] that

$$\sum_{j=1}^{s} \binom{s}{j} j = 2^{s-1}s.$$

Hence, the calculation of L_2 discrepancy using formula (4.6) requires $O(2^{s-1}n^2s)$ operations. This order is very large for large values of s thus confirming that formula (4.6) is not very suitable for computational purposes. We shall now simplify (4.6) to obtain a computationally more suitable expression for the L_2 discrepancy. It will be seen that the use of this alternative expression requires only $O(n^2s)$ operations. In order to obtain this, we will need the following lemma.

Lemma 4.1 *For a given set $S = \{1, 2, \ldots, s\}$ and numbers $a_1, \ldots, a_s$, we have*

$$\sum_{\emptyset \neq \mathbf{u} \subseteq S} \prod_{j \in \mathbf{u}} a_j = \prod_{j=1}^{s} (1 + a_j) - 1.$$

Proof. This lemma may be proved by first considering,

$$\prod_{j=1}^{s} (1 + a_j) - 1 = (1 + a_1)(1 + a_2) \cdots (1 + a_s) - 1.$$

Expanding the right-hand side of this equation gives $2^s - 1$ distinct terms, where each term is a product of i of the a_j and $(s - i)$ 1's for $1 \leq i \leq s$; that is, they are of the form $a_{k_1} a_{k_2} \cdots a_{k_i} 1^{s-i}$. For each value of i, there are $\binom{s}{i}$ such terms. These terms correspond to the terms in the expansion of

$$\sum_{\emptyset \neq \mathbf{u} \subseteq S} \prod_{j \in \mathbf{u}} a_j,$$

hence proving the lemma. □

Using this lemma, we shall now simplify expression (4.6) for the squared L_2 discrepancy. We will consider each of the three terms on the right-hand side of this expression in turn. The first term may be simplified as

$$\sum_{\emptyset \neq \mathbf{u} \subseteq S} \left(\frac{1}{3}\right)^{|\mathbf{u}|} = \prod_{j=1}^{s} \left(1 + \frac{1}{3}\right) - 1 = \left(\frac{4}{3}\right)^{s} - 1, \tag{4.7}$$

followed by the second term

$$-\frac{2}{n}\sum_{\emptyset\neq\mathbf{u}\subseteq S}\sum_{i=0}^{n-1}\prod_{j\in\mathbf{u}}\frac{1}{2}\left(1-t_{i,j}^2\right)=-\frac{2}{n}\sum_{i=0}^{n-1}\sum_{\emptyset\neq\mathbf{u}\subseteq S}\prod_{j\in\mathbf{u}}\frac{1}{2}\left(1-t_{i,j}^2\right)$$
$$=-\frac{2}{n}\sum_{i=0}^{n-1}\left(\prod_{j=1}^{s}\left(1+\frac{1}{2}\left(1-t_{i,j}^2\right)\right)-1\right)=-\frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2}-\frac{t_{i,j}^2}{2}\right)+2, \tag{4.8}$$

and finally the third term

$$\frac{1}{n^2}\sum_{\emptyset\neq\mathbf{u}\subseteq S}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j\in\mathbf{u}}\left[1-\max\left(t_{i,j},t_{k,j}\right)\right]$$
$$=\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\sum_{\emptyset\neq\mathbf{u}\subseteq S}\prod_{j\in\mathbf{u}}\left[1-\max\left(t_{i,j},t_{k,j}\right)\right]$$
$$=\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left(\prod_{j=1}^{s}\left[2-\max\left(t_{i,j},t_{k,j}\right)\right]-1\right)$$
$$=\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[2-\max\left(t_{i,j},t_{k,j}\right)\right]-1. \tag{4.9}$$

Adding (4.7), (4.8) and (4.9), we get a simplified expression for the squared L_2 discrepancy given by

$$D^2(Q)=\left(\frac{4}{3}\right)^s-\frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2}-\frac{t_{i,j}^2}{2}\right)+\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[2-\max\left(t_{i,j},t_{k,j}\right)\right]. \tag{4.10}$$

4.3 Use of reproducing kernel Hilbert spaces to derive the L_2 discrepancy

Reproducing kernel Hilbert spaces have previously been used by Wahba [35] in the analysis of multivariate splines. Recently they have also been used to derive error bounds and formulas for the worst-case integrands. In this section, we shall use them for this latter purpose. In particular, we will use it as an alternative method for the derivation of the L_2 discrepancy given in (4.10). The results given here are based on the work of Sloan and Woźniakowski [34] and that of Hickernell [9].

We first present the theory behind the reproducing kernel Hilbert space approach. Suppose that we have a Hilbert space H of real-valued functions defined over the unit cube $[0,1]^s$. If we denote the inner product on this space by $\langle\cdot,\cdot\rangle$, then the norm induced by it is given by

$$\|f\| = \sqrt{\langle f, f\rangle}.$$

For any $\mathbf{t} \in [0,1]^s$, we define the evaluation functional $\Delta_{\mathbf{t}}$ as

$$\Delta_{\mathbf{t}}(f) = f(\mathbf{t}), \quad \forall f \in H.$$

If $\Delta_{\mathbf{t}}$ is bounded, then by Riesz representation theorem there exists a function K which is defined on $[0,1]^s \times [0,1]^s$ such that

$$\Delta_{\mathbf{t}}(f) = f(\mathbf{t}) = \langle K(\cdot,\mathbf{t}), f\rangle, \quad \forall f \in H, \quad \forall \mathbf{t} \in [0,1]^s.$$

The function K is known as a reproducing kernel. For details concerning reproducing kernels, one may refer to the article by Aronszajn [2].

Once we have the reproducing kernel K for the Hilbert space H, we may express any other linear functional, say δ, in terms of this; that is,

$$\delta(f) = \langle \zeta, f\rangle, \quad \forall f \in H, \quad \text{where} \quad \zeta(\mathbf{t}) = \langle K(\cdot,\mathbf{t}), \zeta\rangle = \delta(K(\cdot,\mathbf{t})). \tag{4.11}$$

Here, ζ is known as the representer for the linear functional δ. In particular, when $\delta = I - Q$, the error of the rule (1.2) may be written as

$$(I-Q)(f) = \langle \eta, f\rangle, \quad \forall f \in H, \quad \text{where} \quad \eta(\mathbf{t}) = (I-Q)(K(\cdot,\mathbf{t})).$$

Then using the Cauchy-Schwarz inequality, the error bound is given by

$$|I(f) - Q(f)| = |\langle \eta, f\rangle| \le \|\eta\|\;\|f\|. \tag{4.12}$$

Equality holds when f is a multiple of the worst case integrand, η. Here, the quantity $\|\eta\|$ is the figure of merit that depends only on the point set that is used in the integration and $\|f\|$ is a measure of the variation of the integrand f. We shall be concerned with the special case of the bound (4.12) for a particular choice of H. When this is the case, the error bound is given by

$$|I(f) - Q(f)| \le D(Q)\|f\|_s,$$

where $\|\cdot\|_s$ is the norm in the Sobolev space (to be defined later). In this section our aim is to show that expression (4.10) for $D(Q)$ may be recovered by using this reproducing kernel Hilbert space approach. In order to do this, we assume that the Hilbert space H is the Sobolev space (for more information on Sobolev spaces, see [1]) of absolutely continuous functions defined by

$$H_s = \{f \in W_2^{(1,1,\ldots,1)}([0,1]^s) : \|f\|_s < \infty\},$$

where

$$\begin{aligned}\|f\|_s &= \left(\sum_{\mathbf{u}\subseteq S}\int_{[0,1]^{|\mathbf{u}|}}\left|\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{t_u}} f(\mathbf{t_u},\mathbf{1})\right|^2 \mathrm{d}\mathbf{t_u}\right)^{1/2}\\ &= \left(|f(\mathbf{1})|^2 + \sum_{\emptyset\neq\mathbf{u}\subseteq S}\int_{[0,1]^{|\mathbf{u}|}}\left|\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{t_u}} f(\mathbf{t_u},\mathbf{1})\right|^2 \mathrm{d}\mathbf{t_u}\right)^{1/2}\end{aligned}$$

and $W_2^{(1,1,\ldots,1)}([0,1]^s)$ is the tensor product,

$$W_2^1([0,1]) \otimes \cdots \otimes W_2^1([0,1]).$$

Here, $W_2^1([0,1])$ are subsets of absolutely continuous functions whose first derivatives belong to $L_2([0,1])$ (the space of Lebesgue square integrable functions on $[0,1]$). The L_2 discrepancy is defined as the worst case error over the unit ball in H_s; that is,

$$D(Q) := \sup_{f\in H_s, \|f\|_s\leq 1} |I(f) - Q(f)|.$$

Moreover, this space has the reproducing kernel (as shown in [34]) given by

$$K_s(\mathbf{v},\mathbf{t}) = \prod_{j=1}^{s}[1+\min(1-v_j, 1-t_j)] = \prod_{j=1}^{s}[(2-\max(v_j,t_j))].$$

Then it follows from (4.11) that the integration functional I may be written in terms of the reproducing kernel as

$$I(f) = \int_{[0,1]^s} f(\mathbf{t})\,\mathrm{d}\mathbf{t} = \langle h, f\rangle_s,$$

where $\langle\cdot,\cdot\rangle_s$ is the inner product on H_s defined as

$$\langle f, g\rangle_s = \sum_{\mathbf{u}\subseteq S}\int_{[0,1]^s}\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{t_u}} f(\mathbf{t_u},\mathbf{1})\,\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{t_u}} g(\mathbf{t_u},\mathbf{1})\,\mathrm{d}\mathbf{t_u}$$

and

$$h(\mathbf{t}) = \int_{[0,1]^s} K_s(\mathbf{v},\mathbf{t})\,\mathrm{d}\mathbf{v}. \tag{4.13}$$

Here, h is the representer of multiple integration and it follows from [34] that

$$\|h\|_s = \|I\| = \left(\int_{[0,1]^{2s}} K_s(\mathbf{v},\mathbf{t})\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{t}\right)^{1/2} = \left(\int_{[0,1]^s}\int_{[0,1]^s} K_s(\mathbf{v},\mathbf{t})\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{t}\right)^{1/2} \tag{4.14}$$

For the quasi-Monte Carlo rule Q, the error in integration may then be written as

$$I(f) - Q(f) = \int_{[0,1]^s} f(\mathbf{t})\,\mathrm{d}\mathbf{t} - \frac{1}{n}\sum_{i=0}^{n-1} f(\mathbf{t}_i) = \left\langle f, h - \frac{1}{n}\sum_{i=0}^{n-1} K_s(\cdot,\mathbf{t}_i)\right\rangle_s,$$

where h is given in (4.13). It then follows from [34] that the L_2 discrepancy is given by

$$D(Q) := \sup_{f\in H_s, \|f\|_s\le 1} |I(f) - Q(f)| = \left\| h - \frac{1}{n}\sum_{i=0}^{n-1} K_s(\cdot,\mathbf{t}_i)\right\|_s.$$

This above equation may be simplified as follows.

$$\begin{aligned} D^2(Q) &= \left\langle h - \frac{1}{n}\sum_{i=0}^{n-1} K_s(\cdot,\mathbf{t}_i),\ h - \frac{1}{n}\sum_{i=0}^{n-1} K_s(\cdot,\mathbf{t}_i)\right\rangle_s \\ &= \langle h, h\rangle_s - \frac{2}{n}\sum_{i=0}^{n-1}\langle h, K_s(\cdot,\mathbf{t}_i)\rangle_s + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\langle K_s(\cdot,\mathbf{t}_i), K_s(\cdot,\mathbf{t}_k)\rangle_s. \end{aligned}$$

Since $\langle h, K(\cdot,\mathbf{t}_i)\rangle_s = h(\mathbf{t}_i)$ and $\langle K(\cdot,\mathbf{t}_i), K(\cdot,\mathbf{t}_k)\rangle_s = K(\mathbf{t}_i,\mathbf{t}_k)$, we have

$$D^2(Q) = \|h\|_s^2 - \frac{2}{n}\sum_{i=0}^{n-1} h(\mathbf{t}_i) + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_s(\mathbf{t}_i,\mathbf{t}_k). \tag{4.15}$$

We may then obtain an expression for $h(\mathbf{t}_i)$ as follows.

$$\begin{aligned} h(\mathbf{t}_i) &= \int_{[0,1]^s} K_s(\mathbf{t},\mathbf{t}_i)\,\mathrm{d}\mathbf{t} = \int_{[0,1]^s}\prod_{j=1}^{s}\left[2 - \max(t_j, t_{i,j})\right]\mathrm{d}\mathbf{t} \\ &= \prod_{j=1}^{s}\int_0^1 \left[2 - \max(t_j, t_{i,j})\right]\mathrm{d}t_j \\ &= \prod_{j=1}^{s}\left[\int_0^{t_{i,j}} (2 - t_{i,j})\,\mathrm{d}t_j + \int_{t_{i,j}}^1 (2 - t_j)\,\mathrm{d}t_j\right] = \prod_{j=1}^{s}\left(\frac{3}{2} - \frac{t_{i,j}^2}{2}\right). \end{aligned} \tag{4.16}$$

Moreover, we see from (4.14) that

$$\begin{aligned} \|h\|_s^2 &= \int_{[0,1]^{2s}} K_s(\mathbf{t}_i,\mathbf{t})\,\mathrm{d}\mathbf{t}_i\,\mathrm{d}\mathbf{t} = \int_{[0,1]^s}\int_{[0,1]^s}\prod_{j=1}^{s}\left[2 - \max(t_{i,j}, t_j)\right]\mathrm{d}\mathbf{t}_i\,\mathrm{d}\mathbf{t} \\ &= \prod_{j=1}^{s}\int_0^1\int_0^1 \left[2 - \max(t_{i,j}, t_j)\right]\mathrm{d}t_{i,j}\,\mathrm{d}t_j \\ &= \prod_{j=1}^{s}\int_0^1\left[\int_0^{t_j} (2 - t_j)\,\mathrm{d}t_{i,j} + \int_{t_j}^1 (2 - t_{i,j})\,\mathrm{d}t_{i,j}\right]\mathrm{d}t_j = \left(\frac{4}{3}\right)^s. \end{aligned} \tag{4.17}$$

Substituting (4.16) and (4.17) into (4.15), we recover the expression for the squared L_2 discrepancy found in (4.10).

4.4 Expected value for Monte Carlo rules

In the next chapter, we shall compare the expected value of the squared discrepancy for Monte Carlo rules with the average discrepancy for other rules having approximately the same number of points. Hence, we need an expression for the expected value for Monte Carlo rules. We shall obtain this below.

Since the points are uniformly distributed on $[0,1]^s$, the expected value for the first two terms of (4.10) is given by

$$\int_{[0,1]^s} \left(\frac{4}{3}\right)^s \mathrm{dt} - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\int_0^1 \left(\frac{3}{2} - \frac{1}{2}t_{i,j}^2\right) \mathrm{d}t_{i,j}$$
$$= \left(\frac{4}{3}\right)^s - 2\left(\frac{3}{2} - \frac{1}{6}\right)^s = -\left(\frac{4}{3}\right)^s. \tag{4.18}$$

Since the third term (the term containing the double summation) of (4.10) has the $\max(t_{i,j}, t_{k,j})$ term, its expected value may be obtained by considering the two possibilities, $i = k$ and $i \neq k$ separately. For the case $i = k$, the points are obviously not independent and the expected value of the third term is given by

$$\frac{n}{n^2}\prod_{j=1}^{s}\int_0^1 (2 - t_{i,j})\,\mathrm{d}t_{i,j} = \frac{1}{n}\left(2 - \frac{1}{2}\right)^s = \frac{1}{n}\left(\frac{3}{2}\right)^s. \tag{4.19}$$

When $i \neq k$, the expected value of this term is

$$\frac{n^2 - n}{n^2}\prod_{j=1}^{s}\int_0^1\int_0^1 [2 - \max(t_{i,j}, t_{k,j})]\,\mathrm{d}t_{i,j}\,\mathrm{d}t_{k,j}. \tag{4.20}$$

In order to compute this, we first note that

$$\int_0^1\int_0^1 \max(t_{i,j}, t_{k,j})\,\mathrm{d}t_{i,j}\,\mathrm{d}t_{k,j} = \int_0^1\int_0^{t_{k,j}} t_{k,j}\;\mathrm{d}t_{i,j}\,\mathrm{d}t_{k,j} + \int_0^1\int_{t_{k,j}}^1 t_{i,j}\;\mathrm{d}t_{i,j}\,\mathrm{d}t_{k,j} = \tfrac{2}{3}. \tag{4.21}$$

It then follows that expression (4.20) may be written as

$$\left(1 - \frac{1}{n}\right)\left(2 - \frac{2}{3}\right)^s = \left(\frac{4}{3}\right)^s - \frac{1}{n}\left(\frac{4}{3}\right)^s.$$

Hence, for Monte Carlo rules having n points, the expected value is given by

$$E_n = -\left(\frac{4}{3}\right)^s + \frac{1}{n}\left(\frac{3}{2}\right)^s + \left(\frac{4}{3}\right)^s - \frac{1}{n}\left(\frac{4}{3}\right)^s = \frac{1}{n}\left[\left(\frac{3}{2}\right)^s - \left(\frac{4}{3}\right)^s\right], \tag{4.22}$$

which recovers the result found in [9].

4.5 The L_2 discrepancy for periodic integrands

In this section we give for quasi-Monte Carlo rules an analogue of the squared L_2 discrepancy (4.10) which may be used to study the error in the case of periodic integrands. This discrepancy will be used in Chapter 7 to compare number-theoretic rules with 2^s copy and Monte Carlo rules in the case of periodic integrands. In order to obtain a discrepancy for periodic integrands, we define the class of functions

$$\bar{H} := \left\{ f : \frac{\partial^{|\mathbf{u}|} f}{\partial \mathbf{t_u}} \in L_2([0,1]^s) \text{ and } \int_0^1 \frac{\partial^{|\mathbf{u}|} f}{\partial \mathbf{t_u}} \, \mathrm{d}t_j = 0, \ \forall j \in \mathbf{u}, \ \forall \mathbf{u} \subseteq S \right\}.$$

It follows from Hickernell [9] that a reproducing kernel for $\bar{H}$ is given by

$$\bar{K}(\mathbf{v}, \mathbf{t}) = \prod_{j=1}^{s} \bar{\eta}_1(v_j, t_j),$$

where

$$\bar{\eta}_1(v_j, t_j) = M + \beta \left[\mu(v_j) + \mu(t_j) - \frac{(-1)}{2} B_2(\{v_j - t_j\}) \right]$$

is the reproducing kernel for the one-dimensional case. Here, $B_2(x) = x^2 - x + 1/6$ is the Bernoulli polynomial and $\mu(t)$ and M satisfy

$$\int_0^1 \mu(t) \, \mathrm{d}t = 0, \quad M = 1 + \beta^2 \int_0^1 \left(\frac{d\mu}{\mathrm{d}t} \right)^2 \mathrm{d}t.$$

Then for the quasi-Monte Carlo rule (1.2), it follows from [9] that the error bound is given by

$$|I(f) - Q(f)| \le \bar{V}(f) \, \bar{D}(Q), \tag{4.23}$$

where $\bar{D}(Q)$ is the L_2 discrepancy given by

$$\begin{aligned} \bar{D}^2(Q) &= M^s - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left[M + \beta^2 \mu(t_{i,j}) \right] \\ &+ \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{s} \left[M + \beta^2 \left(\mu(t_{i,j}) + \mu(t_{k,j}) + \frac{1}{2} B_2(\{t_{i,j} - t_{k,j}\}) \right) \right] \end{aligned} \tag{4.24}$$

and $\bar{V}(f)$ is the appropriate variation of f. It turns out that for our choice of the parameters (given in (4.25) below), this variation is the same as $V(f)$, given in (4.4).

We note from [9] that the quantity P_2 (see (1.14)) may be obtained from expression (4.24) by setting $\mu(t) = 0$ and $\beta = 2\pi$. In order to derive the L_2 discrepancy given in (4.10) for the nonperiodic case, Hickernell [9] chose the parameters,

$$\beta = 1, \quad \mu(t) = \frac{1}{6} - \frac{t^2}{2}, \quad M = \frac{4}{3}, \tag{4.25}$$

in his general expression for the discrepancy of non-periodic integrands. We shall use these same parameters in expression (4.24) to get an analogue of the squared L_2 discrepancy. When this is done, the squared L_2 discrepancy becomes

$$\begin{aligned} \bar{D}^2(Q) = {} & \left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{1}{2}t_{i,j}^2\right) \\ & + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[\frac{7}{4} - \frac{1}{2}\left(t_{i,j}^2 + t_{k,j}^2 - \{t_{i,j} - t_{k,j}\}^2 + \{t_{i,j} - t_{k,j}\}\right)\right]. \end{aligned} \tag{4.26}$$

This L_2 discrepancy may be used in the error analysis of periodic integrands since it appears in the error bound (4.23) and it also allows us to use a goodness criterion that is analogous to the one used in the case of non-periodic integrands. In order to obtain a simplified expression for (4.26), we will need to simplify the quantity

$$\frac{7}{4} - \frac{1}{2}\left(t_{i,j}^2 + t_{k,j}^2 - \{t_{i,j} - t_{k,j}\}^2 + \{t_{i,j} - t_{k,j}\}\right). \tag{4.27}$$

To do this, we shall need the following lemma.

Lemma 4.2 *For numbers x and y such that $0 \le x, y < 1$, we have*

$$\max(x, y) = \frac{1}{2}\left[x^2 + y^2 - 2xy - \{x - y\}^2 + \{x - y\} + x + y\right].$$

Proof. We first note that

$$\{x - y\} = \begin{cases} x - y, & x \ge y, \\ x - y + 1, & x < y. \end{cases}$$

The square of this term may be written as

$$\{x - y\}^2 = \begin{cases} (x - y)^2, & x \ge y, \\ (x - y)^2 + 2(x - y) + 1, & x < y. \end{cases}$$

It then follows that the difference $\{x-y\}^2 - \{x-y\}$ may be written as

$$\{x-y\}^2 - \{x-y\} = \begin{cases} (x-y)^2 - x + y, & x \geq y, \\ (x-y)^2 + x - y, & x < y. \end{cases}$$

This in turn may be written as

$$\{x-y\}^2 - \{x-y\} - x - y = \begin{cases} (x-y)^2 - 2x, & x \geq y, \\ (x-y)^2 - 2y, & x < y. \end{cases}$$

From this it follows that

$$-\{x-y\}^2 + \{x-y\} + x^2 + y^2 + x + y - 2xy = \begin{cases} 2x, & x \geq y, \\ 2y, & x < y. \end{cases}$$

The right-hand side of this equation is just $2\max(x,y)$. Hence the result follows. □

Using this lemma, we may replace the quantity (4.27) in expression (4.26) by

$$\frac{7}{4} + \frac{1}{2}t_{i,j} + \frac{1}{2}t_{k,j} - t_{i,j}t_{k,j} - \max(t_{i,j}, t_{k,j}).$$

Hence for the case of periodic integrands, the L_2 discrepancy for quasi-Monte Carlo rules is given by

$$\begin{aligned} \bar{D}^2(Q) = & \left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{t_{i,j}^2}{2}\right) \\ & + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[\frac{7}{4} + \frac{t_{i,j}}{2} + \frac{t_{k,j}}{2} - t_{i,j}t_{k,j} - \max(t_{i,j}, t_{k,j})\right]. \end{aligned} \tag{4.28}$$

We shall make use of this L_2 discrepancy in Chapter 7 to compare the performance of number-theoretic rules with 2^s copy and Monte Carlo rules in the case of periodic integrands.

Chapter 5

Average discrepancy for optimal vertex-modified number-theoretic rules

5.1 Chapter summary

Recall from Chapter 1 that the vertex-modified rule is given by

$$M(f) = \sum_{i_1=0}^{1} \cdots \sum_{i_s=0}^{1} w_{i_1,\dots,i_s} f(i_1, \dots , i_s) + \frac{1}{n} \sum_{i=1}^{n-1} f\left(\mathbf{t}_i\right). \tag{5.1}$$

For this rule there are obviously many choices for the weights $w_{i_1,\dots,i_s}$. However, it has been shown by Niederreiter and Sloan [25] that the weights may be chosen optimally in the sense that its discrepancy (to be defined later) is minimized. These optimal weights are given by

$$\bar{w}_{i_1,\dots,i_s} = \frac{1}{2^s} - \frac{1}{n} \sum_{i=1}^{n-1} \ell_{i_1,\dots,i_s}(\mathbf{t}_i), \tag{5.2}$$

with

$$\ell_{i_1,\dots,i_s}(t_1, \dots , t_s) = \prod_{j=1}^{s} \left(1 - i_j - (-1)^{i_j} t_j\right), \quad i_j \in \{0, 1\}.$$

Here, $\ell_{i_1,\dots,i_s}$ has the value 1 at the vertex $(i_1, \dots , i_s)$ and the value 0 at all other vertices. Moreover, with this choice of weights M integrates exactly every multilinear polynomial (every polynomial of degree at most 1 in each of its s variables). When the optimal weights are used in M, the resulting rule, denoted by $\overline{M}$, will be referred to as the optimal vertex-modified rule. By taking $\mathbf{t}_i = \{i\mathbf{z}/n\}$ in expression (5.1), we get the vertex-modified number-theoretic rule M_{nt}. Although these vertex-modified number-theoretic rules have been proposed for non-periodic integrands, their potential when compared to normal number-theoretic rules is not clear. In order to investigate this, we derive in Section 5.3 an expression for the average of $D^2(\overline{M}_{\mathrm{nt}})$ (for prime n), where $\overline{M}_{\mathrm{nt}}$ is the optimal vertex-modified number-theoretic rule (vertex-modified number theoretic rule with weights chosen optimally). We shall denote this average by $E_N[D^2(\overline{M}_{\mathrm{nt}})]$, where $N = n - 1 + 2^s$ is the number of function evaluations required by $\overline{M}_{\mathrm{nt}}$. In order to obtain the expression for $E_N[D^2(\overline{M}_{\mathrm{nt}})]$, we derive in Section 5.2 a general expression relating $D^2(\overline{M})$ to $D^2(Q)$ (where Q is the rule given in (1.2)). This expression in turn may be used to write $D^2(\overline{M}_{\mathrm{nt}})$ in terms of $D^2(Q_{\mathrm{nt}})$, the squared L_2 discrepancy of the original number-theoretic rule Q_{nt} given in (1.9). In the final section, Section 5.4, numerical results are given. We present numerical values of $E_N[D^2(\overline{M}_{\mathrm{nt}})]$ together with values of the corresponding average $E_{N'}[D^2(Q_{\mathrm{nt}})]$ for normal number-theoretic rules, where N' is a prime number close to N. These values may also be compared with the expected value for Monte Carlo rules. For reasonable numbers of points, the numerical results indicate that the optimal vertex-modified number-theoretic rules have a smaller average L_2 discrepancy than number-theoretic or Monte Carlo rules when the dimension s is less than 12. The results of this chapter have appeared in Reddy and Joe [29].

5.2 Discrepancy for the optimal vertex-modified rule

In this section we shall obtain an expression for $D^2(\overline{M})$ in terms of $D^2(Q)$. Once we have this relationship, we may substitute $Q = Q_{\mathrm{nt}}$ and $\overline{M} = \overline{M}_{\mathrm{nt}}$ to obtain the result for number-theoretic rules as a special case. This result will be used in the next section to obtain an expression for $E_N[D^2(\overline{M}_{\mathrm{nt}})]$.

The error for the modified rule M given in (5.1) is defined in terms of the local discrepancy (4.2). Niederreiter and Sloan [25] proved that its error satisfies

$$|M(f) - I(f)| \le D(M)V(f), \tag{5.3}$$

where the L_2 discrepancy, $D(M)$, is given by

$$D(M) = \left(\sum_{\emptyset \neq \mathbf{u} \subseteq S} \int_{[0,1]^{|\mathbf{u}|}} \left(g\left(\mathbf{t_u}, \mathbf{1}\right) - c_{\mathbf{u}}\right)^2 \, \mathrm{d}\mathbf{t_u} \right)^{1/2} \tag{5.4}$$

and $V(f)$ is a measure of the variation of f as given in (4.4). In the above expression for $D(M)$, the constants $c_{\mathbf{u}}$ have the values

$$c_{\mathbf{u}} = \frac{1}{n} - \sum_{i_1=0}^{q_1(\mathbf{u})} \cdots \sum_{i_s=0}^{q_s(\mathbf{u})} w_{i_1,\dots,i_s}, \tag{5.5}$$

where $q_k(\mathbf{u}) = 0$ if $k \in \mathbf{u}$ and $q_k(\mathbf{u}) = 1$ otherwise. (In other words, we sum over only the components *not* in $\mathbf{u}$.)

We remark that if we have the general n'-point quadrature rule

$$\sum_{i=0}^{n'-1} w_i f\left(\mathbf{t}_i\right),$$

where w_i is the weight assigned to $\mathbf{t}_i = (t_{i,1}, t_{i,2}, \dots, t_{i,s})$, then it may be shown (for example, by using the techniques found in Hickernell [9]) that the L_2 discrepancy of this rule is given by

$$\left(\frac{4}{3}\right)^s - 2\sum_{i=0}^{n'-1} w_i \prod_{j=1}^{s} \left(\frac{3}{2} - \frac{t_{i,j}^2}{2}\right) + \sum_{i=0}^{n'-1}\sum_{k=0}^{n'-1} w_i w_k \prod_{j=1}^{s} \left[2 - \max\left(t_{i,j}, t_{k,j}\right)\right]. \tag{5.6}$$

Thus with $n' = n - 1 + 2^s$ and a suitable labeling of the quadrature points and weights, this formula may be used to obtain an alternative expression for $D(M)$.

When $M = Q$ (that is, when $w_{0,\dots,0} = 1/n$ and all the other weights $w_{i_1,\dots,i_s}$ are zero), then $c_{\mathbf{u}} = 0$ for all nonempty $\mathbf{u} \subseteq S$ and the error bound (5.3) reduces to the L_2 version of the well-known Koksma-Hlawka inequality (4.1). Thus when $M = Q$, we obtain

$$D(Q) = \left(\sum_{\emptyset \neq \mathbf{u} \subseteq S} \int_{[0,1]^{|\mathbf{u}|}} g^2\left(\mathbf{t_u}, \mathbf{1}\right) \mathrm{d}\mathbf{t_u} \right)^{1/2} \tag{5.7}$$

If the weights are chosen as in (5.2), then it follows from [25] that the corresponding values of $c_{\mathbf{u}}$ are

$$\bar{c}_{\mathbf{u}} = \int_{[0,1]^{|\mathbf{u}|}} g\left(\mathbf{t}_{\mathbf{u}}, \mathbf{1}\right) \mathrm{d}\mathbf{t}_{\mathbf{u}}.$$

It then follows from (5.4) and (5.7) that

$$D^2(\overline{M}) = \sum_{\emptyset \neq \mathbf{u} \subseteq S} \left(\int_{[0,1]^{|\mathbf{u}|}} g^2\left(\mathbf{t}_{\mathbf{u}}, \mathbf{1}\right) \mathrm{d}\mathbf{t}_{\mathbf{u}} - \bar{c}_{\mathbf{u}}^2 \right) = D^2(Q) - \sum_{\emptyset \neq \mathbf{u} \subseteq S} \bar{c}_{\mathbf{u}}^2. \tag{5.8}$$

It is clear from this expression that $D^2(\overline{M}) \leq D^2(Q)$. However, note that $\overline{M}$ requires $n-1+2^s$ function evaluations, whereas Q requires just n function evaluations. Hence, it would not be fair to just compare $D^2(\overline{M})$ with $D^2(Q)$.

We now look at $\bar{c}_{\mathbf{u}}^2$ in more detail. We first note that

$$\int_0^1 I_{t_{i,j} < t_j} \, \mathrm{d}t_j = \int_{t_{i,j}}^1 1 \, \mathrm{d}t_j = 1 - t_{i,j} \quad \text{and} \quad \int_0^1 t_j \, \mathrm{d}t_j = \tfrac{1}{2}.$$

Then using the expression for the local discrepancy given in (4.5) we have

$$\begin{aligned} \bar{c}_{\mathbf{u}}^2 &= \left[\int_{[0,1]^{|\mathbf{u}|}} g\left(\mathbf{t}_{\mathbf{u}}, \mathbf{1}\right) \mathrm{d}\mathbf{t}_{\mathbf{u}} \right]^2 = \left[\frac{1}{n} \sum_{i=0}^{n-1} \prod_{j \in \mathbf{u}} (1 - t_{i,j}) - \prod_{j \in \mathbf{u}} \frac{1}{2} \right]^2 \\ &= \prod_{j \in \mathbf{u}} \frac{1}{4} - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j \in \mathbf{u}} \left(\frac{1}{2} - \frac{t_{i,j}}{2} \right) + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j \in \mathbf{u}} (1 - t_{i,j} - t_{k,j} + t_{i,j} t_{k,j}). \end{aligned}$$

Now recall from Lemma 4.1 that for numbers $a_1, a_2, \ldots, a_s$ and $S = \{1, 2, \ldots, s\}$ we have

$$\sum_{\emptyset \neq \mathbf{u} \subseteq S} \prod_{j \in \mathbf{u}} a_j = \prod_{j=1}^{s} (1 + a_j) - 1.$$

Hence

$$\sum_{\emptyset \neq \mathbf{u} \subseteq S} \bar{c}_{\mathbf{u}}^2 = \left(\frac{5}{4} \right)^s - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{3}{2} - \frac{t_{i,j}}{2} \right) + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{s} (2 - t_{i,j} - t_{k,j} + t_{i,j} t_{k,j}).$$

We then conclude from (5.8) that the squared discrepancy $D^2(\overline{M})$ may be written as

$$\begin{aligned} D^2(\overline{M}) &= D^2(Q) - \left[\left(\frac{5}{4} \right)^s - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{3}{2} - \frac{t_{i,j}}{2} \right) \right. \\ &\qquad \left. + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{s} (2 - t_{i,j} - t_{k,j} + t_{i,j} t_{k,j}) \right]. \end{aligned} \tag{5.9}$$

This expression is computationally more efficient for the calculation of $D^2(\overline{M})$ than the one given in (5.8). This is because use of (5.8) together with (5.5) requires computation of the optimal weights $\bar{w}_{i_1, \ldots, i_s}$ whereas use of this one does not.

5.3 Average L_2 discrepancy for optimal vertex-modified number-theoretic rules

Here we make use of (5.9) with $\overline{M} = \overline{M}_{\mathrm{nt}}$ and $Q = Q_{\mathrm{nt}}$ to derive an expression for $E_N[D^2(\overline{M}_{\mathrm{nt}})]$, the average of $D^2(\overline{M}_{\mathrm{nt}})$ (found from expression (5.9) by taking $t_{i,j} = \{iz_j/n\}$), as defined in the following definition.

Definition 5.1 *For any integer $n \geq 2$, let $N = n - 1 + 2^s$ and let $X = X(n)$ be the set of all $\mathbf{z} \in \mathbb{Z}^s$ whose components z_j are relatively prime to n and satisfy $1 \leq z_j \leq n-1$. The average of the squared discrepancy, $D^2(\overline{M}_{\mathrm{nt}})$, over $\mathbf{z} \in X$ is*

$$E_N[D^2(\overline{M}_{\mathrm{nt}})] := \frac{1}{\varphi(n)^s} \sum_{\mathbf{z} \in X} D^2(\overline{M}_{\mathrm{nt}}),$$

where φ is Euler's function.

We remark here that a computer search for vectors $\mathbf{z}$ that give a small discrepancy is computationally expensive. Thus, having a value for the average discrepancy may be useful in giving a guide as to when a good vector $\mathbf{z}$ has been found.

By using (4.10) or (5.6) with $n' = n$, $w_i = 1/n$, and $t_{i,j} = \{iz_j/n\}$, we see that an explicit expression for $D^2(Q_{\mathrm{nt}})$ is given by

$$\begin{aligned} D^2(Q_{\mathrm{nt}}) &= \left(\frac{4}{3}\right)^s - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{3}{2} - \frac{1}{2}\left\{\frac{iz_j}{n}\right\}^2\right) \\ &\quad + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{s} \left[2 - \max\left(\left\{\frac{iz_j}{n}\right\}, \left\{\frac{kz_j}{n}\right\}\right)\right]. \end{aligned}$$

Using the notation of Definition 5.1 one can define an analogous average of $D^2(Q_{\mathrm{nt}})$ by

$$E_n[D^2(Q_{\mathrm{nt}})] := \frac{1}{\varphi(n)^s} \sum_{\mathbf{z} \in X} D^2(Q_{\mathrm{nt}}). \tag{5.10}$$

Then it was shown in [13] that an expression for this average when n is prime is given by

$$\begin{aligned} E_n[D^2(Q_{\mathrm{nt}})] &= \left(\frac{4}{3}\right)^s + \frac{n-3}{n^2}\left(\frac{3}{2}\right)^s - \frac{2(n-1)}{n}\left(\frac{4}{3} + \frac{1}{12n}\right)^s + \frac{2^s}{n^2} \\ &\quad + \frac{n-1}{n^2} \sum_{k=2}^{n-1} \left(\frac{4}{3} + \frac{1}{12n} + \frac{S(k,n)}{n-1}\right)^s, \end{aligned} \tag{5.11}$$

where the function $S(k,n)$ is the Dedekind sum given by

$$S(k,n) = \sum_{z=1}^{n-1} \frac{z}{n} \left(\left(\frac{kz}{n} \right) \right), \tag{5.12}$$

with

$$((x)) = \begin{cases} 0, & x \in \mathbb{Z}, \\ x - \lfloor x \rfloor - 1/2, & \text{otherwise.} \end{cases}$$

Readers interested in the properties of Dedekind sums should refer to articles such as [27]. Closed form expressions for $S(k,n)$ are not available in the literature. However, the algorithm found in [14] allows $S(k,n)$ to be calculated in at most $O(\log n)$ operations so that the average $E_n[D^2(Q_{\text{nt}})]$ may be calculated in at most $O(n \log n)$ operations. The expression that we obtain for $E_N[D^2(\overline{M}_{\text{nt}})]$ is similar to the one for $E_n[D^2(Q_{\text{nt}})]$ and hence $E_N[D^2(\overline{M}_{\text{nt}})]$ may also be calculated in at most $O(n \log n)$ operations.

In the rest of this chapter, we shall assume that n is prime. Then $\varphi(n) = n-1$ and z_j takes on all values from 1 to $n-1$ inclusive.

It follows from Definition 5.1 and (5.9) (by taking $t_{i,j} = \{iz_j/n\}$) that

$$E_N[D^2(\overline{M}_{\text{nt}})] = E_n[D^2(Q_{\text{nt}})] - \alpha_n,$$

where $E_n[D^2(Q_{\text{nt}})]$ was given in (5.11) and

$$\begin{aligned} \alpha_n &= \left(\frac{5}{4}\right)^s - \frac{2}{n(n-1)^s} \sum_{z_1=1}^{n-1} \cdots \sum_{z_s=1}^{n-1} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{3}{2} - \frac{1}{2} \left\{ \frac{iz_j}{n} \right\} \right) \\ &+ \frac{1}{n^2(n-1)^s} \sum_{z_1=1}^{n-1} \cdots \sum_{z_s=1}^{n-1} \sum_{i,k=0}^{n-1} \prod_{j=1}^{s} \left(2 - \left\{ \frac{iz_j}{n} \right\} - \left\{ \frac{kz_j}{n} \right\} + \left\{ \frac{iz_j}{n} \right\} \left\{ \frac{kz_j}{n} \right\} \right) \\ &= \left(\frac{5}{4}\right)^s - \frac{2}{n} \sum_{i=0}^{n-1} \left(\frac{3}{2} - \frac{1}{2(n-1)} \sum_{z=1}^{n-1} \left\{ \frac{iz}{n} \right\} \right)^s + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} C_{ik}, \end{aligned} \tag{5.13}$$

where

$$C_{ik} = \left(2 - \frac{1}{n-1} \sum_{z=1}^{n-1} \left\{ \frac{iz}{n} \right\} - \frac{1}{n-1} \sum_{z=1}^{n-1} \left\{ \frac{kz}{n} \right\} + \frac{1}{n-1} \sum_{z=1}^{n-1} \left\{ \frac{iz}{n} \right\} \left\{ \frac{kz}{n} \right\} \right)^s. \tag{5.14}$$

To simplify this expression, we shall need the following lemma.

Lemma 5.2 *If n is prime and $1 \le i \le n-1$, then*

$$\frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\} = \frac{1}{2} \quad \text{and} \quad \frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}^2 = \frac{2n-1}{6n}. \tag{5.15}$$

Proof. Since n is prime, we have $\gcd(i,n) = 1$. Then the values of $\{iz/n\}$ for $1 \le i \le n-1$ are just $1/n, \ldots, (n-1)/n$ in some order. Hence by using the familiar sums

$$\sum_{z=1}^{n-1} z = \frac{n(n-1)}{2} \quad \text{and} \quad \sum_{z=1}^{n-1} z^2 = \frac{n(n-1)(2n-1)}{6}, \tag{5.16}$$

the lemma follows. □

By making use of the first sum of Lemma 5.2 we have

$$\left(\frac{3}{2} - \frac{1}{2(n-1)}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\right)^s = \begin{cases} \left(\frac{3}{2}\right)^s, & i = 0, \\ \left(\frac{5}{4}\right)^s, & 1 \le i \le n-1. \end{cases} \tag{5.17}$$

For the C_{ik} given in (5.14), we may use (5.15) to obtain

$$C_{ik} = \begin{cases} 2^s, & i = k = 0, \\ \left(\frac{3}{2}\right)^s, & i = 0,\ k \ne 0 \ \text{ or } \ i \ne 0,\ k = 0, \\ \left(\frac{4}{3} - \frac{1}{6n}\right)^s, & i = k \ne 0, \\ \left(1 + \frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}\right)^s, & \text{otherwise.} \end{cases}$$

Hence

$$\begin{aligned} \sum_{i=0}^{n-1}\sum_{k=0}^{n-1} C_{ik} &= 2^s + 2(n-1)\left(\frac{3}{2}\right)^s + (n-1)\left(\frac{4}{3} - \frac{1}{6n}\right)^s \\ &\quad + \sum_{i=1}^{n-1}\sum_{\substack{k=1 \\ k \ne i}}^{n-1}\left(1 + \frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}\right)^s. \end{aligned} \tag{5.18}$$

In order to simplify this expression, we first consider the simplification of the sum

$$\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}, \tag{5.19}$$

for $1 \leq i, k \leq n-1$ with the restriction that $i \neq k$. We then have a total of $(n-1)(n-2)$ such terms to consider. We first note that

$$\left\{\frac{iz}{n}\right\} = \frac{iz \bmod n}{n}.$$

For z going from 1 to $n-1$, the values $iz \bmod n$ in the above equation are just the values $1, 2, \ldots, n-1$ in some order. Hence for given values of i and m satisfying $1 \leq i, m \leq n-1$, there exists a z, which is dependent on i and m, such that $iz \bmod n = m$. From literature on number theory (for instance, see [26]), we find that this value of z is $mi^{n-2} \bmod n$. We then have

$$\left\{\frac{iz}{n}\right\} = \frac{iz \bmod n}{n} = \frac{m}{n}$$

and

$$\left\{\frac{kz}{n}\right\} = \frac{kz \bmod n}{n} = \frac{(kmi^{n-2} \bmod n) \bmod n}{n} = \frac{k'm \bmod n}{n} = \left\{\frac{k'm}{n}\right\},$$

where $k' = ki^{n-2} \bmod n$. It then follows that

$$\sum_{z=1}^{n-1} \left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\} = \sum_{m=1}^{n-1} \frac{m}{n}\left\{\frac{k'm}{n}\right\}.$$

Since $k \neq i$ and Fermat's little theorem tells us that $i^{n-1} \equiv 1 \pmod{n}$, k' can never be equal to 1. Moreover, we note that for any given value of i, k takes the values $1, 2, \ldots, i-1, i+1, \ldots, n-1$, and for each of these $n-2$ values of k, there is a corresponding distinct value of k'. Now relabeling k' to k and m to z, it follows that for n prime, the double sum in expression (5.18) may be reduced to a single sum; that is,

$$\sum_{i=1}^{n-1} \sum_{\substack{k=1 \\ k \neq i}}^{n-1} \left(1 + \frac{1}{n-1} \sum_{z=1}^{n-1} \left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}\right)^s = (n-1) \sum_{k=2}^{n-1} \left(1 + \frac{1}{n-1} \sum_{z=1}^{n-1} \frac{z}{n}\left\{\frac{kz}{n}\right\}\right)^s. \tag{5.20}$$

Moreover, the single sum inside the parentheses on the right-hand side of this expression may be written as

$$\sum_{z=1}^{n-1} \frac{z}{n}\left(\frac{kz}{n} - \left\lfloor\frac{kz}{n}\right\rfloor - \frac{1}{2} + \frac{1}{2}\right) = S(k, n) + \frac{n-1}{4}, \tag{5.21}$$

where $S(k,n)$ is the Dedekind sum given in (5.12). This last equation, together with (5.20), (5.13), (5.17), and (5.18), yields

$$\begin{aligned}\alpha_n &= \frac{2-n}{n}\left(\frac{5}{4}\right)^s - \frac{2}{n^2}\left(\frac{3}{2}\right)^s + \frac{2^s}{n^2} + \frac{n-1}{n^2}\left(\frac{4}{3}-\frac{1}{6n}\right)^s \\ &\quad + \frac{n-1}{n^2}\sum_{k=2}^{n-1}\left(\frac{5}{4}+\frac{S(k,n)}{n-1}\right)^s.\end{aligned}$$

Since $E_N[D^2(\overline{M}_{\text{nt}})] = E_n[D^2(Q_{\text{nt}})] - \alpha_n$, we can combine this expression for α_n with (5.11) to finally obtain the following result.

Theorem 5.3 *When n is prime, the average value of $D^2(\overline{M}_{\text{nt}})$ for optimal vertex-modified number-theoretic rules is given by*

$$\begin{aligned}E_N[D^2(\overline{M}_{\text{nt}})] &= \left(\frac{4}{3}\right)^s + \frac{n-1}{n^2}\left(\frac{3}{2}\right)^s - \frac{2(n-1)}{n}\left(\frac{4}{3}+\frac{1}{12n}\right)^s \\ &\quad - \frac{n-1}{n^2}\left(\frac{4}{3}-\frac{1}{6n}\right)^s + \frac{n-2}{n}\left(\frac{5}{4}\right)^s \\ &\quad + \frac{n-1}{n^2}\sum_{k=2}^{n-1}\left[\left(\frac{4}{3}+\frac{1}{12n}+\frac{S(k,n)}{n-1}\right)^s - \left(\frac{5}{4}+\frac{S(k,n)}{n-1}\right)^s\right].\end{aligned}$$

In the one-dimensional case, we can substitute $s = 1$ in this last expression and simplify it to obtain $E_{n+1}[D^2(\overline{M}_{\text{nt}})] = 1/(12n^2)$. This value corresponds to the squared L_2 discrepancy of the one-dimensional $(n+1)$-point trapezoidal rule (1.5).

5.4 Numerical results

The optimal vertex-modified number-theoretic rule $\overline{M}_{\text{nt}}$ requires $N = n - 1 + 2^s$ function evaluations and hence it would be natural to compare values of the average $E_N[D^2(\overline{M}_{\text{nt}})]$ for these rules with the average $E_{N'}[D^2(Q_{\text{nt}})]$ for number-theoretic rules (see (5.11)), where N' is a prime number close to N. We may also compare $E_N[D^2(\overline{M}_{\text{nt}})]$ with E_N, the expected value for Monte Carlo rules given in (4.22). These averages for s going from 1 to 20 and $n = 10\,007$, $100\,003$, and $1\,000\,003$ are given in Tables 5.1–5.3. For $s < 12$, the values of $E_N[D^2(\overline{M}_{\text{nt}})]$ in all the three tables are smaller than $E_{N'}[D^2(Q_{\text{nt}})]$, which in turn is smaller than E_N. This suggests that for $s < 12$ these optimal vertex-modified number-theoretic rules are worth considering as an alternative to number-theoretic and Monte Carlo rules.

They are also worth considering for slightly larger values of s (as seen in Tables 5.2 and 5.3) if one is willing to use larger values of n.

We remark that for larger values of s, the numerical results suggest that the average $E_N[D^2(\bar{M}_{\text{nt}})]$ and the expected value E_N have $O(n^{-1})$ and $O(N^{-1})$ behaviour, respectively. Moreover, the average $E_{N'}[D^2(Q_{\text{nt}})]$ has behaviour $O(1/N')$.

Table 5.1: $n = 10,007$

s	$N = n - 1 + 2^s$	N'	$E_N[D^2(\bar{M}_{\text{nt}})]$	$E_{N'}[D^2(Q_{\text{nt}})]$	E_N
1	10008	10009	0.83217E-09	0.33273E-08	0.16653E-04
2	10010	10037	0.20839E-05	0.55190E-05	0.47175E-04
3	10014	10037	0.95974E-05	0.22465E-04	0.10032E-03
4	10022	10037	0.28894E-04	0.61060E-04	0.18978E-03
5	10038	10039	0.71430E-04	0.13851E-03	0.33670E-03
6	10070	10079	0.15713E-03	0.28264E-03	0.57318E-03
7	10134	10139	0.31977E-03	0.53554E-03	0.94675E-03
8	10262	10267	0.61544E-03	0.96201E-03	0.15241E-02
9	10518	10529	0.11358E-02	0.16504E-02	0.23888E-02
10	11030	11047	0.20286E-02	0.26906E-02	0.36181E-02
11	12054	12071	0.35299E-02	0.41255E-02	0.52116E-02
12	14102	14087	0.60126E-02	0.58245E-02	0.69619E-02
13	18198	18191	0.10062E-01	0.73209E-02	0.83815E-02
14	26390	26387	0.16592E-01	0.81006E-02	0.89354E-02
15	42774	42773	0.27017E-01	0.79353E-02	0.84879E-02
16	75542	75541	0.43524E-01	0.70801E-02	0.73743E-02
17	141078	141073	0.69470E-01	0.59300E-02	0.60408E-02
18	272150	272141	0.11000E+00	0.47791E-02	0.47787E-02
19	534294	534283	0.17297E+00	0.37653E-02	0.37065E-02
20	1058582	1058567	0.27034E+00	0.29265E-02	0.28434E-02

Table 5.2: $n = 100,003$

s	$N = n - 1 + 2^s$	N'	$E_N[D^2(\overline{M}_{\mathrm{nt}})]$	$E_{N'}[D^2(Q_{\mathrm{nt}})]$	E_N
1	100004	100019	0.83328E-11	0.33321E-10	0.16666E-05
2	100006	100019	0.20835E-06	0.55510E-06	0.47219E-05
3	100010	100019	0.96057E-06	0.22608E-05	0.10045E-04
4	100018	100019	0.28935E-05	0.61450E-05	0.19017E-04
5	100034	100043	0.71555E-05	0.13933E-04	0.33786E-04
6	100066	100069	0.15745E-04	0.28456E-04	0.57682E-04
7	100130	100151	0.32048E-04	0.54287E-04	0.95819E-04
8	100258	100267	0.61687E-04	0.98680E-04	0.15600E-03
9	100514	100517	0.11385E-03	0.17298E-03	0.24997E-03
10	101026	101027	0.20337E-03	0.29434E-03	0.39502E-03
11	102050	102059	0.35389E-03	0.48805E-03	0.61559E-03
12	104098	104107	0.60281E-03	0.78737E-03	0.94312E-03
13	108194	108203	0.10088E-02	0.12298E-02	0.14098E-02
14	116386	116387	0.16635E-02	0.18343E-02	0.20261E-02
15	132770	132763	0.27087E-02	0.25547E-02	0.27345E-02
16	165538	165533	0.43635E-02	0.32289E-02	0.33652E-02
17	231074	231067	0.69647E-02	0.36192E-02	0.36881E-02
18	362146	362143	0.11028E-01	0.35906E-02	0.35911E-02
19	624290	624277	0.17340E-01	0.32224E-02	0.31721E-02
20	1148578	1148561	0.27100E-01	0.26971E-02	0.26206E-02

Table 5.3: $n = 1,000,003$

s	$N = n - 1 + 2^s$	N'	$E_N[D^2(\overline{M}_{\text{nt}})]$	$E_{N'}[D^2(Q_{\text{nt}})]$	E_N
1	1000004	1000033	0.83333E-13	0.33331E-12	0.16667E-06
2	1000006	1000033	0.20834E-07	0.55550E-07	0.47222E-06
3	1000010	1000033	0.96063E-07	0.22625E-06	0.10046E-05
4	1000018	1000033	0.28939E-06	0.61496E-06	0.19020E-05
5	1000034	1000037	0.71569E-06	0.13944E-05	0.33796E-05
6	1000066	1000081	0.15748E-05	0.28485E-05	0.57716E-05
7	1000130	1000133	0.32055E-05	0.54375E-05	0.95931E-05
8	1000258	1000273	0.61703E-05	0.98950E-05	0.15636E-04
9	1000514	1000537	0.11389E-04	0.17383E-04	0.25112E-04
10	1001026	1001027	0.20343E-04	0.29716E-04	0.39866E-04
11	1002050	1002061	0.35399E-04	0.49701E-04	0.62692E-04
12	1004098	1004117	0.60298E-04	0.81640E-04	0.97776E-04
13	1008194	1008199	0.10091E-03	0.13197E-03	0.15129E-03
14	1016386	1016399	0.16640E-03	0.21002E-03	0.23200E-03
15	1032770	1032793	0.27095E-03	0.32834E-03	0.35154E-03
16	1065538	1065557	0.43648E-03	0.50143E-03	0.52280E-03
17	1131074	1131077	0.69667E-03	0.73908E-03	0.75347E-03
18	1262146	1262143	0.11031E-02	0.10300E-02	0.10304E-02
19	1524290	1524287	0.17345E-02	0.13195E-02	0.12992E-02
20	2048578	2048569	0.27107E-02	0.15120E-02	0.14693E-02

Chapter 6

Average discrepancy for 2^s copy rules

6.1 Chapter summary

In the previous chapter it was seen that for non-periodic integrands, the optimal vertex-modified number-theoretic rules are worth considering as an alternative to the normal number-theoretic and Monte Carlo rules when the dimension s is less than 12. In the case of periodic integrands, it has been shown (see [31]) that the average of P_α (defined in (1.14)) for 2^s copy rules (2^s copies of number-theoretic rules) is smaller than that for normal number-theoretic rules with approximately the same number of points. There is also numerical evidence that 2^s copy rules have smaller values of R (defined in (1.15)) than the number-theoretic rules (see [11]). However, the potential of 2^s copy rules is unknown in the case of integrands which are not periodic. This chapter shall be devoted for this task. We first derive in the next section, an expression for the squared L_2 discrepancy, $D^2(Q_c)$, for 2^s copy rules. We shall then obtain an expression for its average $E_N[D^2(Q_c)]$ in Section 6.3, where $N = 2^s n$ is the number of function evaluations required by Q_c. In Section 6.4, numerical results are given. In this last section the average values of $E_N[D^2(Q_c)]$ are compared with the average $E_{N'}[D^2(Q_{nt})]$ for normal number-theoretic rules. As in the previous chapter, we choose N' to be a prime number close to N. Numerical results show that for values of s from 4 onwards, the average for number-theoretic rules is smaller than that for 2^s copy rules.

6.2 Discrepancy for 2^s copy rules

Recall from Chapter 1 that a 2^s copy of an n-point number-theoretic rule is given by

$$Q_c(f) = \frac{1}{2^s n}\sum_{i=0}^{n-1}\sum_{k_1=0}^{1}\cdots\sum_{k_s=0}^{1} f\left(\frac{1}{2}\left\{\frac{i\mathbf{z}}{n}\right\} + \frac{(k_1, k_2, \ldots, k_s)}{2}\right), \tag{6.1}$$

where $\mathbf{z}$ is a well-chosen integer vector whose components have no factor in common with n. It then follows from (4.1) that the absolute error $|Q_c(f) - I(f)|$ is bounded by

$$|Q_c(f) - I(f)| \leq D(Q_c)V(f),$$

where $D(Q_c)$ is the L_2 discrepancy for the 2^s copy rule and $V(f)$ is the variation of f given in (4.4). We recall from (4.10) that an expression for the squared L_2 discrepancy of a rule Q with N quadrature points $\mathbf{t}_i = (t_{i,1}, \ldots, t_{i,s})$ is given by

$$D^2(Q) = \left(\frac{4}{3}\right)^s - \frac{2}{N}\sum_{i=0}^{N-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{t_{i,j}^2}{2}\right) + \frac{1}{N^2}\sum_{i=0}^{N-1}\sum_{m=0}^{N-1}\prod_{j=1}^{s}\left[2 - \max(t_{i,j}, t_{m,j})\right].$$

For the copy rule (6.1), this expression becomes

$$\begin{aligned} D^2(Q_c) &= \left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\sum_{i=0}^{n-1}\sum_{k_1,\ldots,k_s=0}^{1}\prod_{j=1}^{s}\left[\frac{3}{2} - \frac{1}{2}\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\} + \frac{k_j}{2}\right)^2\right] \\ &+ \frac{1}{4^s n^2}\sum_{i=0}^{n-1}\sum_{k_1,\ldots,k_s=0}^{1}\sum_{m=0}^{n-1}\sum_{l_1,\ldots,l_s=0}^{1}\prod_{j=1}^{s}\left[2 - \max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\} + \frac{k_j}{2}, \frac{1}{2}\left\{\frac{mz_j}{n}\right\} + \frac{l_j}{2}\right)\right]. \end{aligned} \tag{6.2}$$

As usual, the braces indicate that the fractional part of the number is to be taken. To simplify the expression for $D^2(Q_c)$, let us first consider the term

$$\sum_{i=0}^{n-1}\sum_{k_1,\ldots,k_s=0}^{1}\prod_{j=1}^{s}\left[\frac{3}{2} - \frac{1}{2}\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\} + \frac{k_j}{2}\right)^2\right].$$

Taking the sum over k_j for $k_j \in \{0, 1\}$, we obtain

$$\frac{3}{2} - \frac{1}{8}\left\{\frac{iz_j}{n}\right\}^2 + \frac{3}{2} - \frac{1}{2}\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\} + \frac{1}{2}\right)^2 = \frac{23}{8} - \frac{1}{4}\left\{\frac{iz_j}{n}\right\}^2 - \frac{1}{4}\left\{\frac{iz_j}{n}\right\}.$$

Hence the second term in (6.2) simplifies to

$$-\frac{2}{2^s n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{23}{8}-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}^2-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}\right). \tag{6.3}$$

In order to simplify the third term in expression (6.2), we will need to expand the summation over k_j and l_j for $k_j, l_j \in \{0,1\}$. When this is done, the resulting terms are given by

$$\begin{aligned}8 &- \max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}\right)-\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\}+\frac{1}{2},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}\right)\\ &-\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}+\frac{1}{2}\right)-\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\}+\frac{1}{2},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}+\frac{1}{2}\right).\end{aligned} \tag{6.4}$$

An obvious result that will help in the simplification of expression (6.4) is

$$0 \le \frac{1}{2}\left\{\frac{iz_j}{n}\right\} < \frac{1}{2}.$$

Using this result we have

$$\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\}+\frac{1}{2},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}\right)=\frac{1}{2}\left\{\frac{iz_j}{n}\right\}+\frac{1}{2}$$

and

$$\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}+\frac{1}{2}\right)=\frac{1}{2}\left\{\frac{mz_j}{n}\right\}+\frac{1}{2}.$$

Thus expression (6.4) reduces to

$$\frac{13}{2}-\frac{1}{2}\left\{\frac{iz_j}{n}\right\}-\frac{1}{2}\left\{\frac{mz_j}{n}\right\}-2\max\left(\frac{1}{2}\left\{\frac{iz_j}{n}\right\},\frac{1}{2}\left\{\frac{mz_j}{n}\right\}\right). \tag{6.5}$$

The following result then follows from expressions (6.2), (6.3) and (6.5).

Theorem 6.1 *The squared L_2 discrepancy for 2^s copy rules is given by*

$$\begin{aligned}D^2(Q_c) &= \left(\frac{4}{3}\right)^s-\frac{2}{2^s n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{23}{8}-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}^2-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}\right)\\ &+\frac{1}{4^s n^2}\sum_{i=0}^{n-1}\sum_{m=0}^{n-1}\prod_{j=1}^{s}\left[\frac{13}{2}-\frac{1}{2}\left\{\frac{iz_j}{n}\right\}-\frac{1}{2}\left\{\frac{mz_j}{n}\right\}-\max\left(\left\{\frac{iz_j}{n}\right\},\left\{\frac{mz_j}{n}\right\}\right)\right].\end{aligned} \tag{6.6}$$

We remark that this expression is computationally more efficient for the calculation of $D^2(Q_c)$ than the one given in (6.2). In the following section a formula for an average of this quantity will be derived.

6.3 Average L_2 discrepancy for 2^s copy rules

We shall derive a convenient expression for the average of $D^2(Q_c)$, given in (6.6). Analogous to Definition 5.1, the average of $D^2(Q_c)$ may be defined in the following way.

Definition 6.2 *For any integer $n \geq 2$ and $N = 2^s n$, let $X = X(n)$ be the set of all $\mathbf{z} \in \mathbb{Z}^s$ whose components z_j are relatively prime to n and satisfy $1 \leq z_j \leq n-1$. The average of the squared discrepancy $D^2(Q_c)$ for 2^s copy rules, over $\mathbf{z} \in X$ is*

$$E_N[D^2(Q_c)] := \frac{1}{\varphi(n)^s} \sum_{\mathbf{z} \in X} D^2(Q_c).$$

We shall obtain an expression for this average when n is a prime number. In this case, we have $\varphi(n) = n-1$. It then follows from Theorem 6.1 that the average discrepancy for 2^s copy rules is given by

$$\begin{aligned} E_N[D^2(Q_c)] &= \left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\sum_{i=0}^{n-1}\left(\frac{23}{8} - \frac{1/4}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}^2 - \frac{1/4}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\right)^s \\ &\quad + \frac{1}{4^s n^2}\sum_{i=0}^{n-1}\sum_{m=0}^{n-1}\left[\frac{13}{2} - \frac{1/2}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\} - \frac{1/2}{n-1}\sum_{z=1}^{n-1}\left\{\frac{mz}{n}\right\}\right. \\ &\quad \left. - \frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\left\{\frac{iz}{n}\right\},\left\{\frac{mz}{n}\right\}\right)\right]^s. \end{aligned} \tag{6.7}$$

By making use of Lemma 5.2, the expression

$$\left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\sum_{i=0}^{n-1}\left(\frac{23}{8} - \frac{1/4}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}^2 - \frac{1/4}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\right)^s$$

may be written as

$$\left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\left(\frac{23}{8}\right)^s - \frac{2(n-1)}{2^s n}\left(\frac{8}{3} + \frac{1}{24n}\right)^s, \tag{6.8}$$

where the second and the third terms of this last expression arise when $i = 0$ and $1 \leq i \leq n-1$, respectively in the second term of (6.7).

Now by using Lemma 5.2, the term in (6.7) involving the double summation may be simplified to

$$\frac{1}{4^s n^2}\left(\frac{13}{2}\right)^s + \frac{n-1}{4^s n^2}\left(\frac{11}{2}\right)^s + \frac{2(n-1)}{4^s n^2}\left(\frac{23}{4}\right)^s + \frac{1}{4^s n^2}\sum_{i=1}^{n-1}\sum_{\substack{m=1 \\ m\neq i}}^{n-1} T_{im}, \tag{6.9}$$

where T_{im} is given by

$$T_{im} = \left[6 - \frac{1}{n-1} \sum_{z=1}^{n-1} \max \left(\left\{ \frac{iz}{n} \right\}, \left\{ \frac{mz}{n} \right\} \right) \right]^{s}.$$

In the expression given in (6.9), the first term comes from the case $i = m = 0$, the second comes from the case $i = m \neq 0$ and the third one follows from the cases $i = 0, m \neq 0$ and $m = 0, i \neq 0$.

In order to simplify expression (6.9) further, we first replace the index m by k. It then follows from the arguments that lead to (5.20) that

$$\sum_{i=1}^{n-1} \sum_{\substack{k=1 \\ k \neq i}}^{n-1} T_{ik} = (n-1) \sum_{k=2}^{n-1} \left[6 - \frac{1}{n-1} \sum_{z=1}^{n-1} \max \left(\frac{z}{n}, \left\{ \frac{kz}{n} \right\} \right) \right]^{s}. \tag{6.10}$$

In order to simplify the above expression, we will need to simplify

$$\sum_{z=1}^{n-1} \max \left(\frac{z}{n}, \left\{ \frac{kz}{n} \right\} \right).$$

If we set $t_z = z/n$ and $u_z = \{kz/n\}$, then recall from Lemma 4.2 that an expression for $\max(t_z, u_z)$ is given by

$$\max(t_z, u_z) = \frac{1}{2} \left[t_z^2 + u_z^2 - 2t_z u_z - \{t_z - u_z\}^2 + \{t_z - u_z\} + t_z + u_z \right].$$

Hence, we have

$$\sum_{z=1}^{n-1} \max \left(\frac{z}{n}, \left\{ \frac{kz}{n} \right\} \right) = \frac{1}{2} \sum_{z=1}^{n-1} \left[t_z^2 + u_z^2 - 2t_z u_z - \{t_z - u_z\}^2 + \{t_z - u_z\} + t_z + u_z \right]. \tag{6.11}$$

In order to carry out further simplification of this expression, we shall need the following result from [13].

Lemma 6.3 *For a prime number n and some fixed positive integer k satisfying $2 \leq k \leq n-1$, the values of $\{t_z - u_z\}$ are just the fractions $1/n, 2/n, \ldots, (n-1)/n$ in some order for z going from 1 to $n-1$.*

Proof. We first note that

$$t_z - u_z = \frac{z}{n} - \left\{ \frac{kz}{n} \right\} = \frac{z - kz \bmod n}{n}.$$

For some integer m, we may write $kz \bmod n = kz - mn$. When this is done, we have

$$\begin{aligned} t_z - u_z &= \frac{z - kz + mn}{n} = \frac{(1-k)z + mn}{n} \\ &= \frac{nz + (1-k)z + mn - nz}{n} = \frac{(n+1-k)z + (m-z)n}{n} \\ &= \frac{(n+1-k)z}{n} + (m - z). \end{aligned}$$

Since m and z are both integers, so is $m - z$. Therefore,

$$\{t_z - u_z\} = \left\{\frac{(n+1-k)z}{n} + (m-z)\right\} = \left\{\frac{(n+1-k)z}{n}\right\} = \frac{(n+1-k)z \bmod n}{n}.$$

If k is fixed, then for z going from 1 to $n-1$, we see that the values of $(n+1-k)z \bmod n$ are just the integers $1, 2, \ldots, n-1$ taken in some order. In other words, $\{t_z - u_z\}$ are just the fractions $1/n, 2/n, \ldots, (n-1)/n$ taken in some order. □

We note that the values of both $t_z = z/n$ and $u_z = \{kz/n\}$ go through $1/n,\ 2/n, \ldots, (n-1)/n$ in some order for z going from 1 to $n-1$. It then follows from (6.11) and from Lemma 6.3 that for $2 \leq k \leq n-1$,

$$\begin{aligned} \sum_{z=1}^{n-1} \max(t_z, u_z) &= \frac{1}{2}\sum_{z=1}^{n-1}\left[t_z^2 + u_z^2 - \{t_z - u_z\}^2 + \{t_z - u_z\} + t_z + u_z\right] - \sum_{z=1}^{n-1} t_z u_z \\ &= \frac{1}{2}\sum_{z=1}^{n-1}\left[\left(\frac{z}{n}\right)^2 + \left(\frac{z}{n}\right)^2 - \left(\frac{z}{n}\right)^2 + \frac{z}{n} + \frac{z}{n} + \frac{z}{n}\right] - \sum_{z=1}^{n-1} t_z u_z \\ &= \frac{1}{2}\sum_{z=1}^{n-1}\left[\left(\frac{z}{n}\right)^2 + 3\frac{z}{n}\right] - \sum_{z=1}^{n-1} t_z u_z \\ &= \frac{(11n-1)(n-1)}{12n} - \sum_{z=1}^{n-1} t_z u_z. \end{aligned} \tag{6.12}$$

The last step in the above simplification follows from the sums given in (5.16). Now

$$\begin{aligned} \sum_{z=1}^{n-1} t_z u_z &= \sum_{z=1}^{n-1} \frac{z}{n}\left\{\frac{kz}{n}\right\} = \sum_{z=1}^{n-1} \frac{z}{n}\left(\frac{kz}{n} - \left\lfloor\frac{kz}{n}\right\rfloor\right) \\ &= \sum_{z=1}^{n-1} \frac{z}{n}\left(\frac{kz}{n} - \left\lfloor\frac{kz}{n}\right\rfloor - \frac{1}{2} + \frac{1}{2}\right) \\ &= S(k,n) + \frac{1}{2}\sum_{z=1}^{n-1}\frac{z}{n} = S(k,n) + \frac{n-1}{4}, \end{aligned} \tag{6.13}$$

where $S(k,n)$ is the Dedekind sum given in (5.12). Using expression (6.13), (6.12) may be written as

$$\sum_{z=1}^{n-1} \max(t_z, u_z) = \frac{(11n-1)(n-1)}{12n} - S(k,n) - \frac{n-1}{4}.$$

It then follows that for $2 \le k \le n-1$,

$$\frac{1}{n-1}\sum_{z=1}^{n-1} \max\left(\frac{z}{n}, \left\{\frac{kz}{n}\right\}\right) = \frac{11n-1}{12n} - \frac{S(k,n)}{n-1} - \frac{1}{4} = \frac{2}{3} - \frac{1}{12n} - \frac{S(k,n)}{n-1}. \tag{6.14}$$

Hence, by using expressions (6.7), (6.8), (6.9) and (6.10) together with this last expression, we get the following result.

Theorem 6.4 *For n prime, the average L_2 discrepancy for 2^s copy rules is given by*

$$E_N[D^2(Q_c)] = \left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\left(\frac{23}{8}\right)^s - \frac{2(n-1)}{2^s n}\left(\frac{8}{3} + \frac{1}{24n}\right)^s + \frac{1}{4^s n^2}\left(\frac{13}{2}\right)^s$$
$$+\frac{n-1}{4^s n^2}\left(\frac{11}{2}\right)^s + \frac{2(n-1)}{4^s n^2}\left(\frac{23}{4}\right)^s + \frac{n-1}{4^s n^2}\sum_{k=2}^{n-1}\left(\frac{16}{3} + \frac{1}{12n} + \frac{S(k,n)}{n-1}\right)^s.$$

In the one-dimensional case, this expression simplifies to

$$E_{2n}[D^2(Q_c)] = \frac{1}{12n^2}.$$

This value corresponds to the squared L_2 discrepancy for the one-dimensional $2n$-point rectangle rule (1.4).

6.4 Numerical results

The results of some computations are presented in this section. Tables (6.1)–(6.4) gives the average $E_N[D^2(Q_c)]$ for 2^s copy rules together with the average $E_{N'}[D^2(Q_{\rm nt})]$ (see (5.11)) for normal number-theoretic rules for values of s going from 1 to 15 and for $n = 79$, 157, 313 and 619. Here, N' denotes a prime number close to $N = 2^s n$. Numerical results presented in all the four tables clearly show that for values of s from 4 onwards, the average discrepancy for number-theoretic rules is smaller than that for 2^s copy rules. The results given here suggest that 2^s copy rules

Table 6.1: $n = 79$

s	$N = 2^s n$	N'	$E_N[D^2(Q_c)]$	$E_{N'}[D^2(Q_{\text{nt}})]$
1	158	157	0.13353E-04	0.13523E-04
2	316	313	0.82888E-04	0.17825E-03
3	632	631	0.26477E-03	0.34915E-03
4	1264	1259	0.65570E-03	0.48655E-03
5	2528	2521	0.14185E-02	0.54631E-03
6	5056	5051	0.28227E-02	0.56097E-03
7	10112	10111	0.53087E-02	0.53680E-03
8	20224	20219	0.95898E-02	0.48899E-03
9	40448	40433	0.16813E-01	0.42978E-03
10	80896	80863	0.28811E-01	0.36782E-03
11	161792	161783	0.48505E-01	0.30786E-03
12	323584	323581	0.80533E-01	0.25333E-03
13	647168	647161	0.13225E+00	0.20559E-03
14	1294336	1294309	0.21530E+00	0.16491E-03
15	2588672	2588671	0.34812E+00	0.13099E-03

are not as competitive as the number-theoretic rules with approximately the same number of points when dealing with integrands which are not periodic. We remark that these results support Hickernell's comments in [8] that number-theoretic rules tend to be better for integrating functions with large low-order analysis of variance (ANOVA) effects (for information on ANOVA effects, see [8]).

Table 6.2: $n = 157$

s	$N = 2^s n$	N'	$E_N[D^2(Q_c)]$	$E_{N'}[D^2(Q_{\mathrm{nt}})]$
1	314	313	0.33808E-05	0.34024E-05
2	628	619	0.31235E-04	0.89642E-04
3	1256	1249	0.10823E-03	0.17844E-03
4	2512	2503	0.27642E-03	0.24321E-03
5	5024	5023	0.60572E-03	0.27625E-03
6	10048	10039	0.12103E-02	0.28305E-03
7	20096	20089	0.22741E-02	0.27031E-03
8	40192	40189	0.40901E-02	0.24607E-03
9	80384	80369	0.71212E-02	0.21635E-03
10	160768	160757	0.12094E-01	0.18502E-03
11	321536	321509	0.20146E-01	0.15490E-03
12	643072	643061	0.33043E-01	0.12748E-03
13	1286144	1286119	0.53534E-01	0.10345E-03
14	2572288	2572279	0.85878E-01	0.82981E-04
15	5144576	5144569	0.13668E+00	0.65914E-04

Table 6.3: $n = 313$

s	$N = 2^s n$	N'	$E_N[D^2(Q_c)]$	$E_{N'}[D^2(Q_{\mathrm{nt}})]$
1	626	619	0.85061E-06	0.86996E-06
2	1252	1249	0.13241E-04	0.44038E-04
3	2504	2503	0.48860E-04	0.89496E-04
4	5008	5003	0.12750E-03	0.12225E-03
5	10016	10009	0.28180E-03	0.13902E-03
6	20032	20029	0.56459E-03	0.14202E-03
7	40064	40063	0.10600E-02	0.13565E-03
8	80128	80111	0.19008E-02	0.12350E-03
9	160256	160253	0.32936E-02	0.10851E-03
10	320512	320483	0.55591E-02	0.92810E-04
11	641024	640993	0.91906E-02	0.77699E-04
12	1282048	1282033	0.14944E-01	0.63942E-04
13	2564096	2564077	0.23973E-01	0.51891E-04
14	5128192	5128153	0.38036E-01	0.41623E-04
15	10256384	10256369	0.59802E-01	0.33062E-04

Table 6.4: $n = 619$

s	$N = 2^s n$	N'	$E_N[D^2(Q_c)]$	$E_{N'}[D^2(Q_{\mathrm{nt}})]$
1	1238	1237	0.21749E-06	0.21784E-06
2	2476	2473	0.61396E-05	0.22362E-04
3	4952	4951	0.23560E-04	0.45333E-04
4	9904	9901	0.62249E-04	0.61796E-04
5	19808	19801	0.13825E-03	0.70222E-04
6	39616	39607	0.27739E-03	0.71830E-04
7	79232	79231	0.52057E-03	0.68608E-04
8	158464	158449	0.93180E-03	0.62453E-04
9	316928	316919	0.16102E-02	0.54877E-04
10	633856	633833	0.27080E-02	0.46930E-04
11	1267712	1267711	0.44573E-02	0.39288E-04
12	2535424	2535413	0.72104E-02	0.32333E-04
13	5070848	5070847	0.11499E-01	0.26239E-04
14	10141696	10141667	0.18122E-01	0.21047E-04
15	20283392	20283391	0.28279E-01	0.16718E-04

Chapter 7

Average discrepancy for periodic integrands

7.1 Chapter summary

In the numerical integration of periodic integrands over the s-dimensional unit cube, various performance criteria such as P_α (1.14) and R (1.15) have previously been used. When the average of P_α was used to measure the potential of number-theoretic rules against their 2^s copies, it was found that the average values for 2^s copy rules were smaller than those for number-theoretic rules with roughly the same number of points (as shown in [6]). Moreover, there is numerical evidence that 2^s copy rules have smaller values of R than the number-theoretic rules (see [11]). In this chapter, we shall use the L_2 discrepancy, given in (4.28), to study the error in the case of periodic integrands. We shall compare the average of this discrepancy for number-theoretic and 2^s copy rules with the expected value for Monte Carlo rules. In order to carry out such a comparison, we first derive the expected value for Monte Carlo rules in Section 7.2. Then in Section 7.3, we obtain an expression for the average $E_n[\bar{D}^2(Q_{\mathrm{nt}})]$ of number-theoretic rules. In Section 7.4, we derive the discrepancy $\bar{D}^2(Q_{\mathrm{c}})$ for 2^s copy rules and in Section 7.5 an expression for its average $E_N[\bar{D}^2(Q_{\mathrm{c}})]$ is found. Numerical results are given in the final section, Section 7.6.

7.2 Expected value for Monte Carlo rules

For periodic integrands, we recall from (4.28) that the L_2 discrepancy for quasi-Monte Carlo rules with quadrature points $\mathbf{t}_i = (t_{i,1}, \ldots, t_{i,s})$ is given by

$$\bar{D}^2(Q) = \left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{t_{i,j}^2}{2}\right)$$
$$+ \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[\frac{7}{4} + \frac{t_{i,j}}{2} + \frac{t_{k,j}}{2} - t_{i,j}t_{k,j} - \max(t_{i,j}, t_{k,j})\right]. \qquad (7.1)$$

We may use this discrepancy to compare number-theoretic and 2^s copy rules with Monte Carlo rules. In order to do this, we shall need the expected value $\bar{E}_N$ for Monte Carlo rules. First we recall from (4.18) that the expected value for

$$\left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{1}{2}t_{i,j}^2\right)$$

with respect to a uniform distribution is given by

$$\left(\frac{4}{3}\right)^s - 2\left(\frac{3}{2} - \frac{1}{6}\right)^s = -\left(\frac{4}{3}\right)^s.$$

Since the third term in (7.1) involves the $\max(t_{i,j}, t_{k,j})$ term, it follows from (4.19) that the expected value for the third term when $i = k$ is given by

$$\frac{n}{n^2}\left(\frac{7}{4} + \frac{1}{4} + \frac{1}{4} - \frac{1}{3} - \frac{1}{2}\right)^s = \frac{1}{n}\left(\frac{17}{12}\right)^s.$$

When $i \neq k$, it follows from (4.21) that the expected value for this third term is given by

$$\frac{n^2 - n}{n^2}\left(\frac{7}{4} + \frac{1}{4} + \frac{1}{4} - \frac{1}{4} - \frac{2}{3}\right)^s = \left(1 - \frac{1}{n}\right)\left(\frac{4}{3}\right)^s.$$

Hence, the expected value $\bar{E}_N$ for Monte Carlo rules is given by

$$\bar{E}_n = -\left(\frac{4}{3}\right)^s + \frac{1}{n}\left(\frac{17}{12}\right)^s + \left(1 - \frac{1}{n}\right)\left(\frac{4}{3}\right)^s = \frac{1}{n}\left[\left(\frac{17}{12}\right)^s - \left(\frac{4}{3}\right)^s\right]. \qquad (7.2)$$

In the last section, we shall compare this expected value for Monte Carlo rules with the average for number-theoretic and 2^s copy rules with approximately the same number of points.

7.3 Average L_2 discrepancy for number-theoretic rules

For number-theoretic rules it follows from (7.1) that an expression for the L_2 discrepancy is given by

$$\bar{D}^2(Q_{\mathrm{nt}}) = \left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{1}{2}\left\{\frac{iz_j}{n}\right\}^2\right) + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} P_{ik}, \tag{7.3}$$

where

$$P_{ik} = \prod_{j=1}^{s}\left[\frac{7}{4} + \frac{1}{2}\left\{\frac{iz_j}{n}\right\} + \frac{1}{2}\left\{\frac{kz_j}{n}\right\} - \left\{\frac{iz_j}{n}\right\}\left\{\frac{kz_j}{n}\right\} - \max\left(\left\{\frac{iz_j}{n}\right\}, \left\{\frac{kz_j}{n}\right\}\right)\right].$$

The expression for this discrepancy is very similar to the one for the non-periodic case. They only differ in their third term. This reduces the amount of work required in the derivation of its average, which is defined as follows.

Definition 7.1 *For any integer $n \geq 2$, let $X = X(n)$ be the set of all $\mathbf{z} \in \mathbb{Z}^s$ whose components z_j are relatively prime to n and satisfy $1 \leq z_j \leq n-1$. The average of the squared discrepancy $\bar{D}^2(Q_{\mathrm{nt}})$ for number-theoretic rules, over $\mathbf{z} \in X$ is*

$$E_n[\bar{D}^2(Q_{\mathrm{nt}})] := \frac{1}{\varphi(n)^s}\sum_{\mathbf{z}\in X}\bar{D}^2(Q_{\mathrm{nt}}).$$

Here, we shall take n to be prime.

Since the average for the first two terms of expression (7.3) may be obtained from Chapter 5, we only need to find the average of the third term in order to get an expression for the average $E_n[\bar{D}^2(Q_{\mathrm{nt}})]$.

It follows from an argument similar to that by which (5.11) is derived that the quantity,

$$\left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{3}{2} - \frac{1}{2}\left\{\frac{iz_j}{n}\right\}^2\right)$$

has an average given by

$$\beta_n = \left(\frac{4}{3}\right)^s - \frac{2}{n}\left(\frac{3}{2}\right)^s - \frac{2(n-1)}{n}\left(\frac{4}{3} + \frac{1}{12n}\right)^s.$$

We shall now derive the average of the third term

$$\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} P_{ik}. \tag{7.4}$$

Once this average is found, the average $E_n[\bar{D}^2(Q_{\mathrm{nt}})]$ for number-theoretic rules may be obtained by using the formula

$$E_n[\bar{D}^2(Q_{\mathrm{nt}})] = \beta_n + \gamma_n, \tag{7.5}$$

where for a prime number n,

$$\begin{aligned}\gamma_n &= \frac{1}{n^2(n-1)^s}\sum_{z_1=1}^{n-1}\cdots\sum_{z_s=1}^{n-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} P_{ik} \\ &= \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\frac{7}{4}+\frac{1/2}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}+\frac{1/2}{n-1}\sum_{z=1}^{n-1}\left\{\frac{kz}{n}\right\}\right. \\ &\quad \left. -\frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\left\{\frac{iz}{n}\right\},\left\{\frac{kz}{n}\right\}\right)\right]^s.\end{aligned}$$

Using the sums given in Lemma 5.2, the above expression for γ_n simplifies to

$$\begin{aligned}\gamma_n &= \frac{1}{n^2}\left(\frac{7}{4}\right)^s+\frac{n-1}{n^2}\left(\frac{17}{12}+\frac{1}{6n}\right)^s+\frac{2(n-1)}{n^2}\left(\frac{3}{2}\right)^s \\ &+\frac{1}{n^2}\sum_{i=1}^{n-1}\sum_{\substack{k=1\\k\neq i}}^{n-1}\left[\frac{9}{4}-\frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{kz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\left\{\frac{iz}{n}\right\},\left\{\frac{kz}{n}\right\}\right)\right]^s.\end{aligned} \tag{7.6}$$

Here, the first and the second terms come from the cases $i = k = 0$ and $i = k \neq 0$, respectively. The third term arises when $k = 0, i \neq 0$ or $i = 0, k \neq 0$.

It then follows from expressions (5.20) and (6.10) that the term in (7.6) involving the double summation may be written as

$$\frac{(n-1)}{n^2}\sum_{k=2}^{n-1}\left[\frac{9}{4}-\frac{1}{n-1}\sum_{z=1}^{n-1}\frac{z}{n}\left\{\frac{kz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\frac{z}{n},\left\{\frac{kz}{n}\right\}\right)\right]^s.$$

In order to simplify this expression further, we need a few results from the earlier chapters. For the Dedekind sum $S(k,n)$ defined in (5.12), we recall from (5.21) and (6.14) respectively, that

$$\frac{1}{n-1}\sum_{z=1}^{n-1}\frac{z}{n}\left\{\frac{kz}{n}\right\} = \frac{S(k,n)}{n-1}+\frac{1}{4} \tag{7.7}$$

and

$$\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\frac{z}{n},\left\{\frac{kz}{n}\right\}\right)=\frac{2}{3}-\frac{1}{12n}-\frac{S(k,n)}{n-1}. \tag{7.8}$$

Using these results, it then follows that the quantity

$$\left[\frac{9}{4}-\frac{1}{n-1}\sum_{z=1}^{n-1}\frac{z}{n}\left\{\frac{kz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\frac{z}{n},\left\{\frac{kz}{n}\right\}\right)\right]^s$$

may be written as

$$\left[\frac{9}{4}-\left(\frac{S(k,n)}{n-1}+\frac{1}{4}\right)-\left(\frac{2}{3}-\frac{1}{12n}-\frac{S(k,n)}{n-1}\right)\right]^s=\left(\frac{4}{3}+\frac{1}{12n}\right)^s.$$

Hence the average γ_n of the third term (7.4) is given by

$$\frac{1}{n^2}\left(\frac{7}{4}\right)^s+\frac{n-1}{n^2}\left(\frac{17}{12}+\frac{1}{6n}\right)^s+\frac{2(n-1)}{n^2}\left(\frac{3}{2}\right)^s+\frac{(n-1)(n-2)}{n^2}\left(\frac{4}{3}+\frac{1}{12n}\right)^s.$$

The average of number-theoretic rules then follows from (7.5) and is given in the following theorem.

Theorem 7.2 *For a prime number n, the average of the squared L_2 discrepancy (as given in (7.1)) for number-theoretic rules is given by*

$$\begin{aligned} E_n[\bar{D}^2(Q_{\rm nt})] &= \left(\frac{4}{3}\right)^s-\frac{2}{n^2}\left(\frac{3}{2}\right)^s-\frac{(n+2)(n-1)}{n^2}\left(\frac{4}{3}+\frac{1}{12n}\right)^s \\ &\quad +\frac{1}{n^2}\left(\frac{7}{4}\right)^s+\frac{n-1}{n^2}\left(\frac{17}{12}+\frac{1}{6n}\right)^s. \end{aligned} \tag{7.9}$$

We remark that the expression for the average $E_n[D^2(Q_{\rm nt})]$ given in (5.11) contains Dedekind sums and therefore it does not have a closed form. However, this analogous average for the periodic case has a simple closed form.

For the one-dimensional case, we may substitute $s=1$ into expression (7.9) and then simplify it to obtain

$$E_n[\bar{D}^2(Q_{\rm nt})]=\frac{1}{12n^2}.$$

This value corresponds to the squared discrepancy for the one-dimensional n-point rectangle rule.

7.4 Discrepancy for 2^s copy rules

In this section we shall obtain a simple expression for the L_2 discrepancy $\bar{D}^2(Q_c)$ for 2^s copy rules (given in (6.1)) and in the next section its average $E_N[\bar{D}^2(Q_c)]$ will be derived. It follows from (7.1) that $\bar{D}^2(Q_c)$ is given by

$$\begin{aligned}\bar{D}^2(Q_c) = &\left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\sum_{i=0}^{n-1}\sum_{k_1,\dots,k_s=0}^{1}\prod_{j=1}^{s}\left[\frac{3}{2}-\frac{1}{2}\left(w_{i,j}+\frac{k_j}{2}\right)^2\right] \\ &+ \frac{1}{4^s n^2}\sum_{m=0}^{n-1}\sum_{l_1,\dots,l_s=0}^{1}\sum_{i=0}^{n-1}\sum_{k_1,\dots,k_s=0}^{1}\prod_{j=1}^{s}\left[\frac{7}{4}+\frac{1}{2}\left(w_{i,j}+\frac{k_j}{2}\right)+\frac{1}{2}\left(w_{m,j}+\frac{l_j}{2}\right)\right. \\ &\left. - \left(w_{i,j}+\frac{k_j}{2}\right)\left(w_{m,j}+\frac{l_j}{2}\right) - \max\left(w_{i,j}+\frac{k_j}{2}, w_{m,j}+\frac{l_j}{2}\right)\right], \end{aligned} \tag{7.10}$$

where $w_{i,j}$ is given by

$$w_{i,j} = \frac{1}{2}\left\{\frac{iz_j}{n}\right\}. \tag{7.11}$$

In expression (7.10), the braces have been removed since

$$0 \le w_{i,j} + \frac{k_j}{2} < 1 \quad \text{and} \quad 0 \le w_{m,j} + \frac{l_j}{2} < 1.$$

We recall from (6.3) that the expression

$$\frac{2}{2^s n}\sum_{i=0}^{n-1}\sum_{k_1,\dots,k_s=0}^{1}\prod_{j=1}^{s}\left[\frac{3}{2}-\frac{1}{2}\left(w_{i,j}+\frac{k_j}{2}\right)^2\right],$$

with $w_{i,j}$ given in (7.11) has the simplified form

$$\frac{2}{2^s n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{23}{8}-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}^2-\frac{1}{4}\left\{\frac{iz_j}{n}\right\}\right). \tag{7.12}$$

Hence, in order to get a simple expression for the L_2 discrepancy of 2^s copy rules, we only need to consider the third term of (7.10); that is, we will need to consider the simplification of

$$\begin{aligned}&\frac{1}{4^s n^2}\sum_{i=0}^{n-1}\sum_{k_1,\dots,k_s=0}^{1}\sum_{m=0}^{n-1}\sum_{l_1,\dots,l_s=0}^{1}\prod_{j=1}^{s}\left[\frac{7}{4}+\frac{1}{2}\left(w_{i,j}+\frac{k_j}{2}\right)+\frac{1}{2}\left(w_{m,j}+\frac{l_j}{2}\right)\right. \\ &\left. - \left(w_{i,j}+\frac{k_j}{2}\right)\left(w_{m,j}+\frac{l_j}{2}\right) - \max\left(w_{i,j}+\frac{k_j}{2}, w_{m,j}+\frac{l_j}{2}\right)\right].\end{aligned}$$

Expanding this summation over k_j and l_j for $k_j, l_j \in \{0,1\}$, we get the terms

$$\begin{aligned}
&\tfrac{7}{4} + \tfrac{1}{2}w_{i,j} + \tfrac{1}{2}w_{m,j} - w_{i,j}w_{m,j} - \max\left(w_{i,j}, w_{m,j}\right) \\
&+\tfrac{7}{4} + \tfrac{1}{2}(w_{i,j}+1/2) + \tfrac{1}{2}w_{m,j} - \left(w_{i,j}+1/2\right) w_{m,j} - \max\left(w_{i,j}+1/2, w_{m,j}\right) \\
&+\tfrac{7}{4} + \tfrac{1}{2}w_{i,j} + \tfrac{1}{2}(w_{m,j}+1/2) - w_{i,j}\left(w_{m,j}+1/2\right) - \max\left(w_{i,j}, w_{m,j}+1/2\right) \\
&+\tfrac{7}{4} + \tfrac{1}{2}(w_{i,j}+1/2) + \tfrac{1}{2}(w_{m,j}+1/2) - \left(w_{i,j}+1/2\right)\left(w_{m,j}+1/2\right) \\
&- \max\left(w_{i,j}+1/2, w_{m,j}+1/2\right).
\end{aligned}$$

Further simplification gives

$$\begin{aligned}
&8 + 2w_{i,j} + 2w_{m,j} - w_{i,j}w_{m,j} - \max\left(w_{i,j}, w_{m,j}\right) - \left(w_{i,j}+1/2\right) w_{m,j} \\
&- \max\left(w_{i,j}+1/2, w_{m,j}\right) - w_{i,j}\left(w_{m,j}+1/2\right) - \max\left(w_{i,j}, w_{m,j}+1/2\right) \\
&- \left(w_{i,j}+1/2\right)\left(w_{m,j}+1/2\right) - \max\left(w_{i,j}+1/2, w_{m,j}+1/2\right).
\end{aligned}$$

We note that $\max\left(w_{i,j}+1/2, w_{m,j}\right) = w_{i,j}+1/2$ and $\max\left(w_{i,j}, w_{m,j}+1/2\right) = w_{m,j}+1/2$. Hence the above expression simplifies to

$$\frac{25}{4} - 4w_{i,j}w_{m,j} - 2\max\left(w_{i,j}, w_{m,j}\right). \tag{7.13}$$

Replacing $w_{i,j}$ and $w_{m,j}$ by their expressions (see (7.11)), expression (7.13) yields

$$\frac{25}{4} - \left\{\frac{iz_j}{n}\right\}\left\{\frac{mz_j}{n}\right\} - \max\left(\left\{\frac{iz_j}{n}\right\}, \left\{\frac{mz_j}{n}\right\}\right).$$

Using this last expression and the expressions given in (7.10) and (7.12), the following result concerning the L_2 discrepancy for a class of periodic integrands then follows.

Theorem 7.3 *For n prime, the squared L_2 discrepancy (as given in* (7.1)*) for 2^s copy rules, as defined in* (6.1), *is given by*

$$\begin{aligned}
\bar{D}^2(Q_c) = \left(\frac{4}{3}\right)^s - \frac{2}{2^s n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\frac{23}{8} - \frac{1}{4}\left\{\frac{iz_j}{n}\right\}^2 - \frac{1}{4}\left\{\frac{iz_j}{n}\right\}\right) \\
+ \frac{1}{4^s n^2}\sum_{i=0}^{n-1}\sum_{m=0}^{n-1}\prod_{j=1}^{s}\left[\frac{25}{4} - \left\{\frac{iz_j}{n}\right\}\left\{\frac{mz_j}{n}\right\} - \max\left(\left\{\frac{iz_j}{n}\right\}, \left\{\frac{mz_j}{n}\right\}\right)\right].
\end{aligned} \tag{7.14}$$

7.5 Average L_2 discrepancy for 2^s copy rules

Using the notation of Definition 7.1, the average squared discrepancy for 2^s copy rules for periodic integrands is given by

$$E_N[\bar{D}^2(Q_c)] = \frac{1}{(n-1)^s} \sum_{\mathbf{z} \in X} \bar{D}^2(Q_c), \tag{7.15}$$

where n is prime and $N = 2^s n$. We note that the first two terms in the expression (7.14) for the discrepancy of 2^s copy rules are identical to those of its non-periodic counterpart. We recall from (6.8) that the average of this quantity

$$\left(\frac{4}{3}\right)^s - \frac{2}{2^s n} \sum_{i=0}^{n-1} \prod_{j=1}^{s} \left(\frac{23}{8} - \frac{1}{4} \left\{ \frac{iz_j}{n} \right\}^2 - \frac{1}{4} \left\{ \frac{iz_j}{n} \right\} \right)$$

is given by

$$\left(\frac{4}{3}\right)^s - \frac{2}{2^s n} \left(\frac{23}{8}\right)^s - \frac{2(n-1)}{2^s n} \left(\frac{8}{3} + \frac{1}{24n}\right)^s. \tag{7.16}$$

Thus to obtain an expression for the average defined in (7.15), we need to obtain only the average for the third term of (7.14). This is given by

$$\begin{aligned} \lambda_{im} &= \frac{1}{4^s n^2 (n-1)^s} \sum_{z_1=1}^{n-1} \cdots \sum_{z_s=1}^{n-1} \sum_{i=0}^{n-1} \sum_{m=0}^{n-1} \prod_{j=1}^{s} \left[\frac{25}{4} - \left\{ \frac{iz_j}{n} \right\} \left\{ \frac{mz_j}{n} \right\} \right. \\ & \quad \left. - \max \left(\left\{ \frac{iz_j}{n} \right\}, \left\{ \frac{mz_j}{n} \right\} \right) \right]. \end{aligned}$$

Taking the sum over all possible z_j for $1 \le j \le s$, an expression for λ_{im} is given by

$$\frac{1}{4^s n^2} \sum_{i=0}^{n-1} \sum_{m=1}^{n-1} \alpha_{im},$$

where

$$\alpha_{im} = \left[\frac{25}{4} - \frac{1}{n-1} \sum_{z=1}^{n-1} \left\{ \frac{iz}{n} \right\} \left\{ \frac{mz}{n} \right\} - \frac{1}{n-1} \sum_{z=1}^{n-1} \max \left(\left\{ \frac{iz}{n} \right\}, \left\{ \frac{mz}{n} \right\} \right) \right]^s.$$

Using Lemma 5.2, it follows that

$$\alpha_{im} = \begin{cases} \left(\frac{25}{4}\right)^s, & i = m = 0, \\ \left(\frac{23}{4}\right)^s, & i = 0,\ m \neq 0 \quad \text{or} \quad i \neq 0,\ m = 0, \\ \left(\frac{65}{12} + \frac{1}{6n}\right)^s, & i = m \neq 0. \end{cases}$$

For the remaining values of i and m, it follows from (5.20), (6.10), (7.7) and (7.8) that

$$\sum_{i=0}^{n-1}\sum_{\substack{m=1\\m\neq i}}^{n-1}\left[\frac{25}{4}-\frac{1}{n-1}\sum_{z=1}^{n-1}\left\{\frac{iz}{n}\right\}\left\{\frac{mz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\left\{\frac{iz}{n}\right\},\left\{\frac{mz}{n}\right\}\right)\right]^s$$
$$= (n-1)\sum_{m=2}^{n-1}\left[\frac{25}{4}-\frac{1}{n-1}\sum_{z=1}^{n-1}\frac{z}{n}\left\{\frac{mz}{n}\right\}-\frac{1}{n-1}\sum_{z=1}^{n-1}\max\left(\frac{z}{n},\left\{\frac{mz}{n}\right\}\right)\right]^s$$
$$= (n-1)\sum_{m=2}^{n-1}\left[\frac{25}{4}-\left(\frac{S(m,n)}{n-1}+\frac{1}{4}\right)-\left(\frac{2}{3}-\frac{1}{12n}-\frac{S(m,n)}{n-1}\right)\right]^s$$
$$= (n-1)(n-2)\left(\frac{16}{3}+\frac{1}{12n}\right)^s.$$

Hence, λ_{im} may be written as

$$\begin{aligned}\lambda_{im} &= \frac{1}{4^s n^2}\left(\frac{25}{4}\right)^s+\frac{2(n-1)}{4^s n^2}\left(\frac{23}{4}\right)^s+\frac{n-1}{4^s n^2}\left(\frac{65}{12}+\frac{1}{6n}\right)^s\\ &\quad+\frac{(n-1)(n-2)}{4^s n^2}\left(\frac{16}{3}+\frac{1}{12n}\right)^s.\end{aligned}$$

From this last expression for λ_{im} and from the one given in (7.16), we have the following result.

Theorem 7.4 *For prime n, the average of the squared L_2 discrepancy (as given in* (7.1)*) for 2^s copy rules is given by*

$$\begin{aligned}E_N[\bar{D}^2(Q_c)] &= \left(\frac{4}{3}\right)^s-\frac{2}{2^s n}\left(\frac{23}{8}\right)^s-\frac{2(n-1)}{2^s n}\left(\frac{8}{3}+\frac{1}{24n}\right)^s+\frac{1}{4^s n^2}\left(\frac{25}{4}\right)^s\\ &\quad+\frac{2(n-1)}{4^s n^2}\left(\frac{23}{4}\right)^s+\frac{n-1}{4^s n^2}\left(\frac{65}{12}+\frac{1}{6n}\right)^s+\frac{(n-1)(n-2)}{4^s n^2}\left(\frac{16}{3}+\frac{1}{12n}\right)^s.\end{aligned}$$

For the one-dimensional case, this expression reduces to $E_{2n}[\bar{D}^2(Q_c)] = 1/(48n^2)$. This value corresponds to the squared discrepancy for the $2n$-point rectangle rule, given in (1.4).

7.6 Numerical results

Here, we present the results of some computations. Tables 7.1–7.4 gives the average $E_N[\bar{D}^2(Q_c)]$ for 2^s copy rules together with the average $E_{N'}[\bar{D}^2(Q_{nt})]$ (7.9) for number-theoretic rules and the expected value $\bar{E}_N$ (7.2) for Monte Carlo rules.

Table 7.1: $n = 79$

s	$N = 2^s n$	N'	$E_N[\bar{D}^2(Q_c)]$	$E_{N'}[\bar{D}^2(Q_{nt})]$	$\bar{E}_N$
1	158	157	0.33381E-05	0.33808E-05	0.52743E-03
2	316	313	0.19472E-04	0.25802E-04	0.72521E-03
3	632	631	0.61771E-04	0.47546E-04	0.74810E-03
4	1264	1259	0.15381E-03	0.62952E-04	0.68618E-03
5	2528	2521	0.33611E-03	0.70421E-04	0.59023E-03
6	5056	5051	0.67717E-03	0.71356E-04	0.48753E-03
7	10112	10111	0.12910E-02	0.67768E-04	0.39164E-03
8	20224	20219	0.23654E-02	0.61465E-04	0.30828E-03
9	40448	40433	0.42071E-02	0.53809E-04	0.23894E-03
10	80896	80863	0.73133E-02	0.45823E-04	0.18297E-03
11	161792	161783	0.12486E-01	0.38156E-04	0.13875E-03
12	323584	323581	0.21010E-01	0.31215E-04	0.10438E-03
13	647168	647161	0.34940E-01	0.25158E-04	0.78001E-04
14	1294336	1294309	0.57551E-01	0.20022E-04	0.57961E-04
15	2588672	2588671	0.94040E-01	0.15762E-04	0.42862E-04

These values are given for s ranging from 1 to 15 and for $n = 79,\ 157,\ 313$ and 619. We choose N' to be a prime number close to $N = 2^s n$. From all the four tables, we see that for values of s from 4 onwards, the average for number-theoretic rules is smaller than that for 2^s copy and Monte Carlo rules for roughly the same number of points. The trend is similar to that seen for the non-periodic case. The results clearly indicate that the choice of performance criteria is very important as one may reach different conclusions with different choices of the performance criteria. We remark that by making use of ANOVA decomposition, Hickernell [8] pointed out that imbedded rules and Monte Carlo rules tend to be better for integrating functions with large high-order effects, while rank-1 rules tend to be better for integrating functions with large low-order effects.

Table 7.2: $n = 157$

s	$N = 2^s n$	N'	$E_N[\bar{D}^2(Q_c)]$	$E_{N'}[\bar{D}^2(Q_{nt})]$	$\bar{E}_N$
1	314	313	0.84520E-06	0.85061E-06	0.26539E-03
2	628	619	0.63037E-05	0.12143E-04	0.36492E-03
3	1256	1249	0.21163E-04	0.23369E-04	0.37643E-03
4	2512	2503	0.53747E-04	0.31258E-04	0.34528E-03
5	5024	5023	0.11817E-03	0.35115E-04	0.29699E-03
6	10048	10039	0.23794E-03	0.35781E-04	0.24532E-03
7	20096	20089	0.45164E-03	0.34047E-04	0.19707E-03
8	40192	40189	0.82188E-03	0.30892E-04	0.15512E-03
9	80384	80369	0.14495E-02	0.27056E-04	0.12023E-03
10	160768	160757	0.24955E-02	0.23043E-04	0.92069E-04
11	321536	321509	0.42161E-02	0.19197E-04	0.69818E-04
12	643072	643061	0.70162E-02	0.15706E-04	0.52522E-04
13	1286144	1286119	0.11535E-01	0.12659E-04	0.39249E-04
14	2572288	2572279	0.18775E-01	0.10074E-04	0.29165E-04
15	5144576	5144569	0.30312E-01	0.79312E-05	0.21568E-04

Table 7.3: $n = 313$

s	$N = 2^s n$	N'	$E_N[\bar{D}^2(Q_c)]$	$E_{N'}[\bar{D}^2(Q_{nt})]$	$\bar{E}_N$
1	626	619	0.21265E-06	0.21749E-06	0.13312E-03
2	1252	1249	0.22771E-05	0.57870E-05	0.18304E-03
3	2504	2503	0.81035E-05	0.11495E-04	0.18882E-03
4	5008	5003	0.20972E-04	0.15535E-04	0.17319E-03
5	10016	10009	0.46373E-04	0.17565E-04	0.14897E-03
6	20032	20029	0.93322E-04	0.17903E-04	0.12305E-03
7	40064	40063	0.17641E-03	0.17057E-04	0.98848E-04
8	80128	80111	0.31898E-03	0.15490E-04	0.77809E-04
9	160256	160253	0.55804E-03	0.13565E-04	0.60309E-04
10	320512	320483	0.95184E-03	0.11557E-04	0.46181E-04
11	641024	640993	0.15915E-02	0.96280E-05	0.35020E-04
12	1282048	1282033	0.26190E-02	0.78775E-05	0.26345E-04
13	2564096	2564077	0.42545E-02	0.63493E-05	0.19687E-04
14	5128192	5128153	0.68389E-02	0.50531E-05	0.14629E-04
15	10256384	10256369	0.10898E-01	0.39782E-05	0.10818E-04

Table 7.4: $n = 619$

s	$N = 2^s n$	N'	$E_N[\bar{D}^2(Q_c)]$	$E_{N'}[\bar{D}^2(Q_{nt})]$	$\bar{E}_N$
1	1238	1237	0.54372E-07	0.54460E-07	0.67313E-04
2	2476	2473	0.92886E-06	0.28660E-05	0.92555E-04
3	4952	4951	0.34657E-05	0.57698E-05	0.95477E-04
4	9904	9901	0.90982E-05	0.78244E-05	0.87574E-04
5	19808	19801	0.20203E-04	0.88640E-05	0.75328E-04
6	39616	39607	0.40640E-04	0.90460E-05	0.62222E-04
7	79232	79231	0.76591E-04	0.86207E-05	0.49983E-04
8	158464	158449	0.13783E-03	0.78297E-05	0.39344E-04
9	316928	316919	0.23966E-03	0.68585E-05	0.30495E-04
10	633856	633833	0.40585E-03	0.58429E-05	0.23352E-04
11	1267712	1267711	0.67311E-03	0.48680E-05	0.17708E-04
12	2535424	2535413	0.10978E-02	0.39832E-05	0.13322E-04
13	5070848	5070847	0.17661E-02	0.32105E-05	0.99549E-05
14	10141696	10141667	0.28094E-02	0.25551E-05	0.73972E-05
15	20283392	20283391	0.44272E-02	0.20116E-05	0.54703E-05

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