Constructive approaches to quasi-Monte Carlo methods for multiple integration

A thesis presented to

The University of Waikato

in fulfilment of the thesis requirement

for the degree of

Doctor of Philosophy

by

Frances Y. Kuo

The University of Waikato

Te Whare Wānanga o Waikato

The University of Waikato

August, 2002

Abstract

Recently, quasi-Monte Carlo methods have been successfully used for approximating multiple integrals in hundreds of dimensions in mathematical finance, and were significantly more efficient than Monte Carlo methods.

To understand the apparent success of quasi-Monte Carlo methods for multiple integration, one popular approach is to study worst-case error bounds in weighted function spaces in which the importance of the variables is moderated by some sequences of weights. Ideally, a family of quasi-Monte Carlo methods in some weighted function space should be strongly tractable. Strong tractability means that the minimal number of quadrature points n needed to reduce the initial error by a factor of ε is bounded by a polynomial in ε^{-1} independently of the dimension d. Several recent publications show the existence of lattice rules that satisfy the strong tractability error bounds in weighted Korobov spaces of periodic integrands and weighted Sobolev spaces of non-periodic integrands. However, those results were non-constructive and thus give no clues as to how to actually construct these lattice rules.

In this thesis, we focus on the construction of quasi-Monte Carlo methods that are strongly tractable. We develop and justify algorithms for the construction of lattice rules that achieve strong tractability error bounds in weighted Korobov and Sobolev spaces. The parameters characterizing these lattice rules are found 'component-by-component': the $(d+1)$-th components are obtained by successive 1-dimensional searches, with the previous d components kept unchanged. The cost of these algorithms vary from $O(nd^2)$ to $O(n^3d^2)$ operations. With currently available technology, they allow construction of rules easily with values of n up to several million and dimensions d up to several hundred.

Acknowledgements

First of all, I would like to thank my supervisor Dr Stephen Joe, without whom none of this would be possible. Stephen has been a great mentor and a true friend throughout the years. He has taught me much about the art of research. His kind encouragement and tolerance of my ignorance are all gratefully appreciated.

Heartfelt thanks are given to The University of Waikato and The Federation of University Women for providing scholarships that gave me financial support during the time of my study. I would also like to express my appreciation to the Department of Mathematics for providing me with a good research environment. The support from all the staff and fellow students in the department are gratefully acknowledged, especially Dr Ian Hawthorn, for those rewarding conversations.

Next I would like to convey my gratitude to Professor Ian Sloan for the opportunities to collaborate with him. I also appreciate very much the chance to visit him in Sydney where several valuable discussions took place. Ian is truly an expert and I have learned so much from him.

Finally, I would like to thank my husband, Roger, and my whole family for being there for me always whether I am up or down. Most of all, I thank my parents from the bottom of my heart for their endless love and unconditional support throughout my life.

Contents

Chapter 1

Introduction

Quasi-Monte Carlo methods have recently attracted much attention due to their efficiency in approximating multiple integrals in mathematical finance (see [27]). In this chapter, we first give a general introduction to the problem and then outline the contents of each chapter.

1.1 QMC rules for multiple integration

We want to approximate the d-dimensional integral

$$I_d(f) = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{1.1}$$

of functions f belonging to a normed linear space H_d. Quasi-Monte Carlo (QMC) rules are equal-weight quadrature rules of the form

$$Q_{n,d}(f) = \frac{1}{n}\sum_{i=0}^{n-1} f(\boldsymbol{x}_i), \tag{1.2}$$

where $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ are n quadrature points in $[0,1]^d$ chosen in some deterministic way. We will assume that function evaluation is well-defined for functions in H_d.

The general questions we want to ask are: how large does n need to be to ensure a good approximation? And how fast does the minimal number of points required for a given accuracy rise as the dimension d increases? Clearly the answers to these questions depend on the function space, how we choose the quadrature points, and what we mean by a good approximation.

Worst-case error

We define the 'worst-case error' of $Q_{n,d}$ in H_d by its worst-case performance over the unit ball of H_d (with norm $\|\cdot\|_d$):

$$e_{n,d} := \sup\{|I_d(f) - Q_{n,d}(f)| : f \in H_d, \|f\|_d \le 1\}.$$

We also define the initial approximation $Q_{0,d}$ to be 0, so that the initial worst-case error is

$$e_{0,d} := \sup\{|I_d(f)| : f \in H_d, \|f\|_d \le 1\}.$$

Tractability

The tractability of linear multivariate problems has been studied in various works such as [24], [34], [40], and [41]. Here we are interested in the tractability of multiple integration.

For $\varepsilon \in (0,1)$, let $n_{\min}(\varepsilon, d)$ denote the minimal number of points n required such that

$$e_{n,d} \le \varepsilon\, e_{0,d},$$

that is, to reduce the worst-case error from its initial value by a factor of ε.

Following [35], we say that a family $\{Q_{n,d}\}$ of QMC rules is 'tractable' in the space H_d if and only if there exist non-negative C, p and q such that

$$n_{\min}(\varepsilon, d) \le C\varepsilon^{-p} d^q \quad \forall \varepsilon \in (0,1),\, \forall d \ge 1. \tag{1.3}$$

We say that a family $\{Q_{n,d}\}$ of QMC rules is 'strongly tractable' in the space H_d if and only if (1.3) holds with $q = 0$. In this case, the infima of the number p is called the 'ε-exponent' of strong tractability for $\{Q_{n,d}\}$.

We say that multiple integration in the space H_d is 'QMC tractable' (or 'strongly QMC tractable') if and only if there exists a family of QMC rules $\{Q_{n,d}\}$ which is tractable (or strongly tractable) in the space H_d.

1.2 Some families of QMC rules

From this point on, we will consider a family of QMC rules to be 'good' in some function space if it is strongly tractable. Here we introduce some families of QMC rules that we will consider in this thesis.

Lattice rules

A d-dimensional integration lattice, $\mathcal{L}$, is a discrete subset of $\mathbb{R}^d$ which is closed under addition and subtraction, and which contains $\mathbb{Z}^d$ as a subset. Lattice rules are QMC rules where the quadrature points $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ are all the points of an integration lattice $\mathcal{L} \subset \mathbb{R}^d$ that lie in the half-open unit cube $[0,1)^d$. The number of distinct quadrature points in a lattice rule is known as the 'order' of the rule.

It is shown in [32] that every lattice rule can be written as a multiple sum of the form

$$Q_{n,d}(f) = \frac{1}{n} \sum_{i_1=0}^{n_1-1} \sum_{i_2=0}^{n_2-1} \cdots \sum_{i_t=0}^{n_t-1} f\left(\left\{ i_1 \frac{\boldsymbol{z}_1}{n_1} + i_2 \frac{\boldsymbol{z}_2}{n_2} + \cdots + i_t \frac{\boldsymbol{z}_t}{n_t} \right\}\right),$$

where $n = n_1 \cdots n_t$ and for each i satisfying $1 \leq i \leq t$, $\boldsymbol{z}_i \in \mathbb{Z}^d$ has no factor in common with n_i. Here and for the rest of the thesis, the braces around a vector indicate that we take the fractional part of each component of the vector. The minimal number of sums required to write a lattice rule as a multiple sum is know as the 'rank' of the lattice rule. More details on lattice rules can be found in the book [29] by Sloan and Joe.

Rank-1 lattice rules

When we take t in the multiple sum to be 1, we obtain rank-1 lattice rules, which are QMC rules of the form

$$Q_{n,d}(f) = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{ \frac{i\boldsymbol{z}}{n} \right\}\right), \tag{1.4}$$

where $\boldsymbol{z} \in \mathbb{Z}^d$ is the 'generating vector' having no factor in common with n. Rank-1 lattice rules are often referred to as number-theoretic rules as their accuracy is related to the number-theoretic properties of n and the components of $\boldsymbol{z}$. They are also known as the method of good lattice points in some of the literature.

It is usual to restrict $\boldsymbol{z}$ to the set $\mathcal{Z}_n^d$ where

$$\mathcal{Z}_n := \{1 \le z \le n-1 : \gcd(z,n) = 1\}. \tag{1.5}$$

The set $\mathcal{Z}_n$ has $\phi(n)$ elements, where ϕ is Euler's function. When n is a prime number, the set $\mathcal{Z}_n$ is

$$\mathbb{Z}_n := \{1, 2, \ldots, n-1\}.$$

Intermediate-rank lattice rules

We will consider some intermediate-rank lattices rules of the form

$$Q_{n,d,copy(\ell,r)}(f) = \frac{1}{\ell^r n} \sum_{m_r=0}^{\ell-1} \cdots \sum_{m_1=0}^{\ell-1} \sum_{i=0}^{n-1} f\left(\left\{\frac{i\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell}\right\}\right), \tag{1.6}$$

where $\ell \ge 1$, $\gcd(\ell, n) = 1$ and $0 \le r \le d$. When $r = 0$ and/or $\ell = 1$, the rule is an n-point rank-1 lattice rule. For $r \ge 1$, it is a rank-r lattice rule with $N = \ell^r n$ quadrature points.

These rules can in fact be obtained by 'copying' some n-point d-dimensional rank-1 lattice rules ℓ times in each of the first r dimensions. We shall call $\boldsymbol{z}$ the 'generating vector' of the intermediate-rank lattice rule.

Shifted QMC rules

A 'shifted' QMC rule corresponding to the QMC rule (1.2) is

$$Q_{n,d}(f; \Delta) = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\{\boldsymbol{x}_i + \boldsymbol{\Delta}\}\right),$$

where $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ are the quadrature points from the rule (1.2) and $\boldsymbol{\Delta} \in \mathbb{R}^d$ is the 'shift'. Clearly it is sufficient to restrict the shift to the range $[0, 1)^d$.

Shifted rank-1 lattice rules are examples of shifted QMC rules:

$$Q_{n,d}(f;\Delta) = \frac{1}{n}\sum_{i=0}^{n-1} f\left(\left\{\frac{iz}{n} + \Delta\right\}\right), \tag{1.7}$$

where, as before, $\boldsymbol{z} \in \mathcal{Z}_n^d$ is the generating vector and $\boldsymbol{\Delta} \in [0,1)^d$ is the shift. We shall see in later chapters the advantages of having a shift.

1.3 About this thesis

This thesis is devoted to the construction of good QMC rules, and in particular, lattice rules. The generating vectors and/or the shifts are constructed 'component-by-component': the $(d+1)$-th components are obtained by successive 1-dimensional searches, with the previous d components kept unchanged.

We consider integrands in two function spaces: the weighted Korobov spaces of periodic functions and the weighted Sobolev spaces of non-periodic functions. Both these spaces are tensor-product reproducing kernel Hilbert spaces. In Chapter 2, we first look at the properties of such spaces. We then consider in detail weighted Korobov and Sobolev spaces, and how general QMC rules perform in these spaces.

In Chapter 3, we consider rank-1 lattice rules in weighted Korobov spaces. We first show the existence of good rank-1 lattice rules when the number of points n is a prime number. We then develop and justify a component-by-component algorithm for constructing the generating vectors of such rules. This work was done in collaboration with Sloan and Joe. The material was part of an early draft of the paper [30].

In Chapter 4, we consider shifted rank-1 lattice rules in weighted Sobolev spaces. We show that there exists a good pair of generating vector and the shift when n is prime, and such a pair can be constructed by a similar component-by-component algorithm as in weighted Korobov spaces. This work was done in collaboration with Sloan and Joe. The material in this chapter is in the paper [30].

We have assumed in Chapters 3 and 4 that n is a prime number. In Chapter 5, we use a more complicated analysis and show that the results can be generalized to any composite value of n. The material in this chapter, which was done in collaboration with Joe, is in the paper [20].

In Chapter 6, we consider randomly shifted rank-1 lattice rules in weighted Sobolev spaces. We show that good generating vectors can be constructed component-by-component, but instead of constructing the shifts component-by-component, we generate shifts randomly to reduce the cost of the construction and to allow error estimation. This work was done in collaboration with Sloan and Joe. The material in this chapter is in the paper [31].

In Chapter 7, we consider intermediate-rank lattice rules formed by copying rank-1 lattice rules. We show that the generating vector of a good intermediate-rank lattice rule can be constructed component-by-component. Our theory also indicates that, in some cases, the resulting rules are better than rank-1 lattice rules with roughly the same number of points. The material in this chapter has been written up as a paper jointly with Joe.

To further reduce the cost of the construction, we consider in Chapter 8 randomly shifted rank-1 lattice rules where the number of points n is a product of two distinct primes p and q. We show that the generating vectors can be constructed component-by-component based on the decomposition $n = pq$. The material in this chapter has been written up as a joint paper with Dick.

All the constructions given till now are guaranteed to achieve $O(n^{-\frac{1}{2}})$ convergence. It is known from [36] that under appropriate conditions on the weights, there exist rules which achieve the optimal rate of convergence $O(n^{-\frac{\alpha}{2}+\delta})$ for any $\delta > 0$ in weighted Korobov spaces with parameter $\alpha > 1$, or $O(n^{-1+\delta})$ for any $\delta > 0$ in weighted Sobolev spaces. In Chapter 9 we show that the rules constructed by the component-by-component algorithms in fact achieve the optimal rate of convergence in the corresponding weighted function spaces. The material in this chapter has been presented at the 2001 Oberwolfach workshop: Numerical Integration and its Complexity. The paper [19] for this work has been submitted to the special issue of Journal of Complexity.

In Chapter 10, we outline some numerical experiments that have been carried out based on the component-by-component algorithms given in the previous chapters. We present some interesting results from the comparison of rules constructed using different algorithms.

The final chapter, Chapter 11, is quite different from other chapters in the thesis. We consider QMC rules constructed by Sobol's quasi-random generator. Currently available software allows the construction up to only 40 dimensions. We first give an overview of the steps required for their construction and then derive a systematic method which generates the parameters required for the construction of Sobol' sequences to 1111 dimensions or higher. Moreover, the resulting sequences satisfy Sobol's so-called Property A. This joint work with Joe is in the paper [16].

Chapter 2

Weighted Korobov and Sobolev Spaces

We consider in this thesis integrands from weighted Korobov spaces of periodic functions and weighted Sobolev spaces of non-periodic functions. These spaces, which are tensor product reproducing kernel Hilbert spaces, have been considered previously in various papers such as [11], [12], [25], [35], and [36].

In this chapter, we first discuss the general theory of such spaces. We then give the attributes for the weighted Korobov and Sobolev spaces in detail.

2.1 QMC rules in reproducing kernel Hilbert spaces

In this section, we give the properties of reproducing kernel Hilbert spaces and the worst-case error expressions for QMC rules.

2.1.1 Reproducing kernel Hilbert spaces

A reproducing kernel Hilbert space, H_d, of functions on $[0,1]^d$, is a Hilbert space in which point evaluation

$$T_{\boldsymbol{y}}(f) = f(\boldsymbol{y}) \quad \text{for all } \boldsymbol{y} \in [0,1]^d,$$

is a bounded linear functional on H_d.

Reproducing kernel

Let $\langle \cdot, \cdot \rangle_d$ denote the inner product and $\| \cdot \|_d$ denote the norm in the space H_d. By the Riesz representation theorem, there exists a unique function $K_d(\cdot, \boldsymbol{y}) \in H_d$ such that for all $\boldsymbol{y} \in [0,1]^d$,

$$T_{\boldsymbol{y}}(f) = f(\boldsymbol{y}) = \langle f, K_d(\cdot, \boldsymbol{y}) \rangle_d, \qquad \text{for all } f \in H_d.$$

The function $K_d(\boldsymbol{x}, \boldsymbol{y})$, the representer of $T_{\boldsymbol{y}}$, is known as the 'reproducing kernel' of the Hilbert space H_d. For any other bounded linear functional T on H_d, the representer $\tilde{T}$ satisfying $T(f) = \langle f, \tilde{T} \rangle_d$ is given by

$$\tilde{T}(\boldsymbol{y}) = \langle \tilde{T}, K_d(\cdot, \boldsymbol{y}) \rangle_d = T(K_d(\cdot, \boldsymbol{y})). \tag{2.1}$$

Any real-valued reproducing kernel $K_d(\boldsymbol{x}, \boldsymbol{y})$ has the symmetry property

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = K_d(\boldsymbol{y}, \boldsymbol{x}) \qquad \text{for all } \boldsymbol{x}, \boldsymbol{y} \in [0,1]^d.$$

Also,

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = \langle K_d(\boldsymbol{x}, \cdot), K_d(\boldsymbol{y}, \cdot) \rangle_d \qquad \text{for all } \boldsymbol{x}, \boldsymbol{y} \in [0,1]^d.$$

We shall make use of these properties of $K_d(\boldsymbol{x}, \boldsymbol{y})$ without further comment. Full details on reproducing kernels can be found in [3].

Shift-invariant kernel

Following [9] and [11], a reproducing kernel is said to be 'shift-invariant' if it has the property

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = K_d(\{\boldsymbol{x} + \boldsymbol{\Delta}\}, \{\boldsymbol{y} + \boldsymbol{\Delta}\}) \qquad \text{for all } \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\Delta} \in [0,1]^d. \tag{2.2}$$

It can be easily verified that (2.2) is equivalent to

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = K_d(\{\boldsymbol{x} - \boldsymbol{y}\}, \boldsymbol{0}) \qquad \text{for all } \boldsymbol{x}, \boldsymbol{y} \in [0,1]^d. \tag{2.3}$$

As in [9] and [11], associated with any reproducing kernel $K_d(\boldsymbol{x}, \boldsymbol{y})$ is a shift-invariant kernel given by

$$K_d^*(\boldsymbol{x}, \boldsymbol{y}) = \int_{[0,1]^d} K_d(\{\boldsymbol{x} + \boldsymbol{\Delta}\}, \{\boldsymbol{y} + \boldsymbol{\Delta}\}) \, \mathrm{d}\boldsymbol{\Delta}. \tag{2.4}$$

Tensor product spaces

Following [41], a tensor product space $H_d = H_1^{(1)} \otimes \cdots \otimes H_1^{(d)}$ of d 1-dimensional Hilbert spaces $H_1^{(1)}, \ldots, H_1^{(d)}$ is the completion of linear combinations of tensor products $f_1 \otimes \cdots \otimes f_d$ with $f_j \in H_1^{(j)}$ for each $1 \le j \le d$, that is, H_d consists of functions of the form

$$f(\boldsymbol{x}) = \sum_{k_1=1}^{\infty} \cdots \sum_{k_d=1}^{\infty} \left(c_{k_1,\ldots,k_d} \prod_{j=1}^{d} \eta_{k_j}^{(j)}(x_j) \right),$$

where $c_{k_1,\ldots,k_d}$ are real coefficients such that

$$\sum_{k_1=1}^{\infty} \cdots \sum_{k_d=1}^{\infty} c_{k_1,\ldots,k_d}^2 < \infty,$$

and for each $1 \le j \le d$, $\{\eta_k^{(j)}\}_{k=1}^{\infty}$ forms an orthonormal basis for $H_1^{(j)}$.

It turned out that (see [24]) if each $H_1^{(j)}$ is a reproducing kernel Hilbert space and the inner product of H_d is defined in a certain way, then H_d has a reproducing kernel given by the product of the 1-dimensional kernels. This result is summarized in the following lemma:

Lemma 2.1 *Let $H_d = H_1^{(1)} \otimes \cdots \otimes H_1^{(d)}$ where, for each $1 \le j \le d$, $H_1^{(j)}$ is a reproducing kernel Hilbert space with kernel $K_1^{(j)}$ and inner product $\langle \cdot, \cdot \rangle_1^{(j)}$. Suppose the inner product of H_d is defined for $f(\boldsymbol{x}) = \prod_{j=1}^{d} f_j(x_j)$ and $g(\boldsymbol{x}) = \prod_{j=1}^{d} g_j(x_j)$ with $f_j, g_j \in H_1^{(j)}$ as*

$$\langle f, g \rangle_d := \prod_{j=1}^{d} \langle f_j, g_j \rangle_1^{(j)}.$$

Then the reproducing kernel for H_d is

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = \prod_{j=1}^{d} K_1^{(j)}(x_j, y_j).$$

Proof. For any $f \in H_d$, by the linearity of inner product and the property of $K_1^{(j)}$, we have

$$\begin{aligned} \langle f, K_d(\cdot, \boldsymbol{y}) \rangle_d &= \sum_{k_1=1}^{\infty} \cdots \sum_{k_d=1}^{\infty} \left(c_{k_1,\ldots,k_d} \prod_{j=1}^{d} \langle \eta_{k_j}^{(j)}, K_1^{(j)}(\cdot, y_j) \rangle_1^{(j)} \right) \\ &= \sum_{k_1=1}^{\infty} \cdots \sum_{k_d=1}^{\infty} \left(c_{k_1,\ldots,k_d} \prod_{j=1}^{d} \eta_{k_j}^{(j)}(y_j) \right) = f(\boldsymbol{y}). \end{aligned}$$

Thus K_d is the reproducing kernel for H_d as claimed. □

2.1.2 Worst-case errors of QMC rules

Let f be any function in the Hilbert space H_d with real-valued reproducing kernel $K_d(\boldsymbol{x}, \boldsymbol{y})$. We approximate the d-dimensional integral (1.1) with an n-point QMC rule (1.2). Clearly $Q_{n,d}$ is a bounded linear functional on H_d (since point evaluation is a bounded linear functional on H_d). We will assume that I_d is also a bounded linear functional on H_d. From (2.1), the representers of I_d and $Q_{n,d}$ are given by

$$h_d(\boldsymbol{y}) = I_d(K_d(\cdot, \boldsymbol{y})) = \int_{[0,1]^d} K_d(\boldsymbol{x}, \boldsymbol{y})\, \mathrm{d}\boldsymbol{x}$$

and

$$\varsigma_{n,d}(\boldsymbol{y}) = Q_{n,d}(K_d(\cdot, \boldsymbol{y})) = \frac{1}{n}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i, \boldsymbol{y}),$$

respectively, where $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ are the quadrature points. The representer of the quadrature error $I_d(f) - Q_{n,d}(f)$ is then given by

$$\xi_{n,d}(\boldsymbol{y}) = h_d(\boldsymbol{y}) - \varsigma_{n,d}(\boldsymbol{y}),$$

and hence

$$I_d(f) - Q_{n,d}(f) = \langle f, \xi_{n,d} \rangle_d.$$

By the Cauchy-Schwarz inequality,

$$|I_d(f) - Q_{n,d}(f)| = |\langle f, \xi_{n,d} \rangle_d| \leq \|f\|_d \|\xi_{n,d}\|_d,$$

with equality being achieved when f is a multiple of $\xi_{n,d}$.

Let $e_{n,d}(P_{n,d}, K_d)$ denote the worst-case error of a QMC rule with the set of points $P_{n,d} = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}\}$ in a reproducing kernel Hilbert space with kernel K_d. We conclude from the definition of worst-case error that

$$e_{n,d}(P_{n,d}, K_d) = \|\xi_{n,d}\|_d = \left\| \int_{[0,1]^d} K_d(\boldsymbol{x}, \cdot)\, \mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i, \cdot) \right\|_d \tag{2.5}$$

and that the initial worst-case error is simply

$$e_{0,d}(K_d) = \left\| \int_{[0,1]^d} K_d(\boldsymbol{x}, \cdot)\, \mathrm{d}\boldsymbol{x} \right\|_d. \tag{2.6}$$

The expressions for these errors in terms of the reproducing kernel K_d are given in the following lemma.

Lemma 2.2 *We have*

$$e_{0,d}^2(K_d) = \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}$$

and

$$\begin{aligned} e_{n,d}^2(P_{n,d},K_d) &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^d} K_d(\boldsymbol{x}_i,\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \\ &\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\boldsymbol{x}_i,\boldsymbol{x}_k). \end{aligned}$$

Proof. We have from (2.6) that

$$\begin{aligned} e_{0,d}^2(K_d) = \left\| \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} \right\|_d^2 &= \left\langle \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x}, \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} \right\rangle_d \\ &= \int_{[0,1]^{2d}} \langle K_d(\boldsymbol{x},\cdot), K_d(\boldsymbol{y},\cdot)\rangle_d \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}. \end{aligned}$$

Now it follows from (2.5) that

$$\begin{aligned} &e_{n,d}^2(P_{n,d},K_d) \\ &= \left\| \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i,\cdot) \right\|_d^2 \\ &= \left\langle \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i,\cdot), \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i,\cdot) \right\rangle_d \\ &= \left\langle \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x}, \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x} \right\rangle_d \\ &\quad -\frac{2}{n}\sum_{i=0}^{n-1}\left\langle \int_{[0,1]^d} K_d(\boldsymbol{x},\cdot)\,\mathrm{d}\boldsymbol{x}, K_d(\boldsymbol{x}_i,\cdot) \right\rangle_d + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\langle K_d(\boldsymbol{x}_i,\cdot), K_d(\boldsymbol{x}_k,\cdot)\rangle_d \\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^d} K_d(\boldsymbol{x}_i,\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\boldsymbol{x}_i,\boldsymbol{x}_k). \end{aligned}$$

This completes the proof. □

Now we present three important results from [9]. First, as we shall see in the next result, the expressions for the errors are simpler when the reproducing kernel is shift-invariant (see (2.2)).

Lemma 2.3 *If K_d is shift-invariant, then*

$$e_{0,d}^2(K_d) = \int_{[0,1]^d} K_d(\boldsymbol{x}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{x}$$

and

$$e_{n,d}^2(P_{n,d}, K_d) = -\int_{[0,1]^d} K_d(\boldsymbol{x}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\{\boldsymbol{x}_i - \boldsymbol{x}_k\}, \boldsymbol{0}).$$

Proof. Since K_d is shift-invariant, using (2.3) and a change of variable $\boldsymbol{u} = \{\boldsymbol{x} - \boldsymbol{y}\}$, we obtain

$$\begin{aligned}
\int_{[0,1]^{2d}} K_d(\boldsymbol{x}, \boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} &= \int_{[0,1]^{2d}} K_d(\{\boldsymbol{x} - \boldsymbol{y}\}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\
&= \int_{[0,1]^{2d}} K_d(\boldsymbol{u}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{y} \\
&= \int_{[0,1]^d} K_d(\boldsymbol{u}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{u}.
\end{aligned}$$

and

$$\int_{[0,1]^d} K_d(\boldsymbol{x}_i, \boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \int_{[0,1]^d} K_d(\{\boldsymbol{x}_i - \boldsymbol{y}\}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{y} = \int_{[0,1]^d} K_d(\boldsymbol{u}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{u}$$

The result now follows by substituting these expressions into Lemma 2.2. □

Recall that there is a shift-invariant kernel associated with any kernel. According to the lemma below, the mean (over all possible shifts) square worst-case error of a shifted QMC rule given by some arbitrary kernel is the square worst-case error of the original unshifted QMC rule given by the associated shift-invariant kernel.

Lemma 2.4 *Given a QMC rule $Q_{n,d}$ with the set of quadrature points $P_{n,d} = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}\}$, let $P_{n,d}(\boldsymbol{\Delta}) := \{\{\boldsymbol{x}_i + \boldsymbol{\Delta}\} : 0 \le i \le n-1\}$ denote the set of quadrature points for a shifted QMC rule corresponding to the rule $Q_{n,d}$. If K_d^* denote the associated shift-invariant kernel of the kernel K_d, then*

$$\int_{[0,1]^d} e_{n,d}^2(P_{n,d}(\boldsymbol{\Delta}), K_d)\,\mathrm{d}\boldsymbol{\Delta} = e_{n,d}^2(P_{n,d}, K_d^*).$$

Proof. We see from Lemma 2.2 that

$$\begin{aligned}
&\int_{[0,1]^d} e^2_{n,d}(P_{n,d}(\boldsymbol{\Delta}), K_d)\,\mathrm{d}\boldsymbol{\Delta} \\
&= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^{2d}} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}\},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\Delta} \\
&\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^d} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}\},\{\boldsymbol{x}_k+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}.
\end{aligned}$$

With a change of variable $\boldsymbol{x} = \{\boldsymbol{x}_i + \boldsymbol{\Delta}\}$, we have

$$\int_{[0,1]^{2d}} K_d(\{\boldsymbol{x}_i+\Delta\},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\Delta} = \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y},$$

which leads to

$$\begin{aligned}
&\int_{[0,1]^d} e^2_{n,d}(P_{n,d}(\boldsymbol{\Delta}), K_d)\,\mathrm{d}\boldsymbol{\Delta} \\
&= -\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^d} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}\},\{\boldsymbol{x}_k+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}.
\end{aligned}$$

Now we have from Lemma 2.3 that

$$e^2_{n,d}(P_{n,d}, K_d^*) = -\int_{[0,1]^d} K_d^*(\boldsymbol{x},\boldsymbol{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d^*(\{\boldsymbol{x}_i-\boldsymbol{x}_k\},\boldsymbol{0}).$$

With (2.4) and a change of variable, we have

$$\int_{[0,1]^d} K_d^*(\boldsymbol{x},\boldsymbol{0})\,\mathrm{d}\boldsymbol{x} = \int_{[0,1]^{2d}} K_d(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta}\,\mathrm{d}\boldsymbol{x} = \int_{[0,1]^{2d}} K_d(\boldsymbol{u},\boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta}\,\mathrm{d}\boldsymbol{u},$$

and from (2.3)

$$K_d^*(\{\boldsymbol{x}_i-\boldsymbol{x}_k\},\boldsymbol{0}) = K_d^*(\boldsymbol{x}_i,\boldsymbol{x}_k) = \int_{[0,1]^d} K_d(\{\boldsymbol{x}_i+\Delta\},\{\boldsymbol{x}_k+\Delta\})\,\mathrm{d}\boldsymbol{\Delta},$$

and these lead to

$$\begin{aligned}
&e^2_{n,d}(P_{n,d}, K_d^*) \\
&= -\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^d} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}\},\{\boldsymbol{x}_k+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta} \\
&= \int_{[0,1]^d} e^2_{n,d}(P_{n,d}(\boldsymbol{\Delta}), K_d)\,\mathrm{d}\boldsymbol{\Delta},
\end{aligned}$$

which completes the proof. □

Finally, we define the mean square worse-case error taken over all quadrature points:

$$E_{n,d}(K_d) := \int_{[0,1]^{nd}} e^2_{n,d}\left(P_{n,d}, K_d\right) \mathrm{d}\boldsymbol{x}_0 \cdots \mathrm{d}\boldsymbol{x}_{n-1}.$$

We shall call this the 'QMC mean' throughout the thesis. An expression for the QMC mean in terms of the reproducing kernel K_d is given in the next lemma.

Lemma 2.5 *We have*

$$E_{n,d}(K_d) = \frac{1}{n}\left(\int_{[0,1]^d} K_d(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right).$$

Moreover, if K_d is shift-invariant, then

$$E_{n,d}(K_d) = \frac{1}{n}\left(K_d(\boldsymbol{0},\boldsymbol{0}) - \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right).$$

Proof. We have from Lemma 2.2 that

$$\begin{aligned} e^2_{n,d}\left(P_{n,d}, K_d\right) &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^d} K_d(\boldsymbol{x}_i,\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \\ &\quad + \frac{1}{n^2}\sum_{i=0}^{n-1} K_d(\boldsymbol{x}_i,\boldsymbol{x}_i) + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{\substack{k=0\\k\neq i}}^{n-1} K_d(\boldsymbol{x}_i,\boldsymbol{x}_k). \end{aligned}$$

It follows from this and the definition of $E_{n,d}(K_d)$ that

$$\begin{aligned} &E_{n,d}(K_d) \\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^{2d}} K_d(\boldsymbol{x}_i,\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}_i \\ &\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\int_{[0,1]^d} K_d(\boldsymbol{x}_i,\boldsymbol{x}_i)\,\mathrm{d}\boldsymbol{x}_i + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{\substack{k=0\\k\neq i}}^{n-1}\int_{[0,1]^{2d}} K_d(\boldsymbol{x}_i,\boldsymbol{x}_k)\,\mathrm{d}\boldsymbol{x}_i\,\mathrm{d}\boldsymbol{x}_k \\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - 2\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ &\quad + \frac{1}{n}\int_{[0,1]^d} K_d(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \frac{n-1}{n}\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ &= \frac{1}{n}\left(\int_{[0,1]^d} K_d(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right). \end{aligned}$$

If K_d is shift-invariant, then it follows from (2.3) that

$$\int_{[0,1]^d} K_d(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{[0,1]^d} K_d(\boldsymbol{0},\boldsymbol{0})\,\mathrm{d}\boldsymbol{x} = K_d(\boldsymbol{0},\boldsymbol{0}).$$

This completes the proof. □

2.2 Weighted Korobov spaces

Weighted Korobov spaces are tensor product reproducing kernel Hilbert spaces of periodic functions. These spaces have been considered previously in [11], [12], and [36]. An unweighted version has also been considered in [33].

2.2.1 The 1-dimensional case

First of all let us have a look at the 1-dimensional Korobov space. The reproducing kernel Hilbert space $H_{1,\beta,\gamma}$ is the space of 1-periodic complex-valued absolutely integrable functions defined on [0,1] with absolutely convergent Fourier series. The inner product in $H_{1,\beta,\gamma}$ is defined by

$$\langle f, g\rangle_{1,\beta,\gamma} = \beta^{-1}\hat{f}(0)\overline{\hat{g}(0)} + \gamma^{-1} \sum_{h=-\infty}^{\infty}{}' \; |h|^{\alpha}\hat{f}(h)\overline{\hat{g}(h)},$$

where $\alpha > 1$ is a fixed smoothness parameter characterizing the rate of decay of the Fourier coefficients

$$\hat{f}(h) = \int_0^1 e^{-2\pi i h x} f(x)\,\mathrm{d}x, \quad h \in \mathbb{Z},$$

and $\beta, \gamma > 0$ are real parameters (the 'weights'). The prime on the sum indicates that the $h = 0$ term is to be omitted. The norm in the space $H_{1,\beta,\gamma}$ is

$$\|f\|_{1,\beta,\gamma} = \left(\beta^{-1}|\hat{f}(0)|^2 + \gamma^{-1} \sum_{h=-\infty}^{\infty}{}' \; |h|^{\alpha}|\hat{f}(h)|^2\right)^{\frac{1}{2}}$$

We remark that β is taken to be 1 in both [12] and [36].

The expression for the reproducing kernel is given in the following lemma.

Lemma 2.6 *The reproducing kernel for the space $H_{1,\beta,\gamma}$ is*

$$K_{1,\beta,\gamma}(x, y) = \beta + \gamma \sum_{h=-\infty}^{\infty}{}' \; \frac{e^{2\pi i h(x-y)}}{|h|^{\alpha}}.$$

Proof. Since the Fourier expansion of any function g is

$$g(x) = \hat{g}(0) + \sum_{h=-\infty}^{\infty}{}' \; \hat{g}(h)e^{2\pi i h x},$$

we see from the definition of $K_{1,\beta,\gamma}$ that

$$\hat{K}_{1,\beta,\gamma}(h,y) = \begin{cases} \beta, & \text{if } h = 0, \\ \gamma \dfrac{e^{-2\pi i h y}}{|h|^{\alpha}}, & \text{if } h \neq 0. \end{cases}$$

For any given $y \in [0,1]$,

$$\begin{aligned} \langle f, K_{1,\beta,\gamma}(\cdot,y)\rangle_1 &= \beta^{-1}\hat{f}(0)\overline{\hat{K}_{1,\beta,\gamma}(0,y)} + \gamma^{-1}\sum_{h=-\infty}^{\infty}{}' |h|^{\alpha}\hat{f}(h)\overline{\hat{K}_{1,\beta,\gamma}(h,y)} \\ &= \beta^{-1}\hat{f}(0)\beta + \gamma^{-1}\sum_{h=-\infty}^{\infty}{}' |h|^{\alpha}\hat{f}(h)\gamma\frac{e^{2\pi i h y}}{|h|^{\alpha}} \\ &= \hat{f}(0) + \sum_{h=-\infty}^{\infty}{}' \hat{f}(h)e^{2\pi i h y} \\ &= f(y), \end{aligned}$$

which proves that $K_{1,\beta,\gamma}$ is the reproducing kernel. □

2.2.2 The d-dimensional case

Now we define our d-dimensional weighted Korobov space. Suppose we have two positive sequences $\boldsymbol{\beta} = \{\beta_j\}$ and $\boldsymbol{\gamma} = \{\gamma_j\}$ satisfying

$$\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots .$$

We define the d-dimensional weighted Korobov space $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ as the tensor product

$$H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} := H^{(1)}_{1,\beta_1,\gamma_1} \otimes H^{(2)}_{1,\beta_2,\gamma_2} \otimes \cdots \otimes H^{(d)}_{1,\beta_d,\gamma_d}$$

of d different 1-dimensional weighted Korobov spaces with different weights. The ratios of the weights are chosen to be non-increasing to moderate the ordering of the coordinate directions, so that the rate of change is greatest in the x_1 direction, less great in the x_2 direction, and so on.

For $f(\boldsymbol{x}) = \prod_{j=1}^{d} f_j(x_j)$ and $g(\boldsymbol{x}) = \prod_{j=1}^{d} g_j(x_j)$ with $f_j, g_j \in H^{(j)}_{1,\beta_j,\gamma_j}$, we define their inner product in $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ as in Lemma 2.1 by $\langle f,g\rangle_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} := \prod_{j=1}^{d}\langle f_j, g_j\rangle^{(j)}_{1,\beta_j,\gamma_j}$. From this it is possible to show that the inner product for any general $f, g \in$

$H_{d,\beta,\gamma}$ is given by

$$\langle f,g\rangle_{d,\beta,\gamma} = \sum_{\boldsymbol{h}\in\mathbb{Z}^d} \left(\hat{f}(\boldsymbol{h})\overline{\hat{g}(\boldsymbol{h})} \prod_{j=1}^{d} r_\alpha(\beta_j,\gamma_j,h_j) \right),$$

where

$$r_\alpha(\beta,\gamma,h) = \begin{cases} \beta^{-1}, & \text{if } h=0, \\ \gamma^{-1}|h|^\alpha, & \text{if } h\neq 0, \end{cases}$$

and

$$\hat{f}(\boldsymbol{h}) = \int_{[0,1]^d} e^{-2\pi i \boldsymbol{h}\cdot\boldsymbol{x}} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

The norm in $H_{d,\beta,\gamma}$ is

$$\|f\|_{d,\beta,\gamma} = \left[\sum_{\boldsymbol{h}\in\mathbb{Z}^d} \left(|\hat{f}(\boldsymbol{h})|^2 \prod_{j=1}^{d} r_\alpha(\beta_j,\gamma_j,h_j) \right) \right]^{\frac{1}{2}}$$

Moreover, it follows from Lemma 2.1 that the reproducing kernel in $H_{d,\beta,\gamma}$ is

$$K_{d,\beta,\gamma}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d} K_{1,\beta_j,\gamma_j}(x_j,y_j) = \prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_j-y_j)}}{|h|^\alpha} \right). \tag{2.7}$$

We remark that $K_{d,\beta,\gamma}$ is shift-invariant.

2.2.3 QMC rules in weighted Korobov spaces

The expressions for the errors of QMC rules in weighted Korobov spaces are given in the next lemma.

Lemma 2.7 *We have*

$$e_{0,d}^2(K_{d,\beta,\gamma}) = \prod_{j=1}^{d} \beta_j$$

and

$$e_{n,d}^2(P_{n,d},K_{d,\beta,\gamma}) = -\prod_{j=1}^{d}\beta_j + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_{i,j}-x_{k,j})}}{|h|^\alpha} \right).$$

Proof. Since $K_{d,\beta,\gamma}$ is shift-invariant, it follows from Lemma 2.3 that

$$e_{0,d}^2(K_{d,\beta,\gamma}) = \int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x},\boldsymbol{0})\,\mathrm{d}\boldsymbol{x}$$

and

$$
\begin{aligned}
& e_{n,d}^2(P_{n,d}, K_{d,\beta,\gamma}) \\
= & -\int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x}, \mathbf{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_{d,\beta,\gamma}(\{\boldsymbol{x}_i - \boldsymbol{x}_k\}, \mathbf{0}) \\
= & -\int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x}, \mathbf{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi \mathrm{i} h(x_{i,j}-x_{k,j})}}{|h|^\alpha}\right).
\end{aligned}
$$

We have

$$
\begin{aligned}
\int_0^1 K_{1,\beta,\gamma}(x,0)\,\mathrm{d}x &= \int_0^1 \left(\beta + \gamma \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi \mathrm{i} hx}}{|h|^\alpha}\right)\mathrm{d}x \\
&= \beta + \gamma \sum_{h=-\infty}^{\infty}{}' \frac{1}{|h|^\alpha}\int_0^1 e^{2\pi \mathrm{i} hx}\,\mathrm{d}x = \beta,
\end{aligned}
$$

where in the last step we have used the fact that for $h \neq 0$,

$$
\int_0^1 e^{2\pi \mathrm{i} hx}\,\mathrm{d}x = \frac{1}{2\pi \mathrm{i} h}\left(e^{2\pi \mathrm{i} h} - e^0\right) = 0.
$$

Thus

$$
\int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x}, \mathbf{0})\,\mathrm{d}\boldsymbol{x} = \prod_{j=1}^{d}\int_0^1 K_{1,\beta_j,\gamma_j}(x_j, 0)\,\mathrm{d}x_j = \prod_{j=1}^{d}\beta_j.
$$

This completes the proof. □

The Fourier expansion of B_α, the Bernoulli polynomial of degree α, is given by (see [29]),

$$
B_\alpha(x) = \frac{(-1)^{\frac{\alpha}{2}+1}\alpha!}{(2\pi)^\alpha}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi \mathrm{i} hx}}{h^\alpha}, \quad x \in [0,1]. \tag{2.8}
$$

Thus, we can express the infinite sum in the last term of the square worst-case error as

$$
\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi \mathrm{i} h(x_{i,j}-x_{k,j})}}{|h|^\alpha} = \frac{(2\pi)^\alpha}{(-1)^{\frac{\alpha}{2}+1}\alpha!}B_\alpha\left(\{x_{i,j} - x_{k,j}\}\right).
$$

In practice, it is usual to take $\alpha \geq 2$ to be an even integer.

The expression for the QMC mean $E_{n,d}\left(K_{d,\beta,\gamma}\right)$ in weighted Korobov spaces is given in the following lemma.

Lemma 2.8 *We have*

$$
E_{n,d}\left(K_{d,\beta,\gamma}\right) = \frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) - \prod_{j=1}^{d}\beta_j\right),
$$

where

$$\zeta(\alpha) = \sum_{h=1}^{\infty} h^{-\alpha}, \quad \alpha > 1,$$

is the Riemann zeta function.

Proof. It follows from Lemma 2.5 that

$$E_{n,d}(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}) = \frac{1}{n}\left(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\mathbf{0},\mathbf{0}) - \int_{[0,1]^{2d}} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right),$$

where $K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is as given in (2.7). We have

$$K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\mathbf{0},\mathbf{0}) = \prod_{j=1}^{d}\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{1}{|h|^{\alpha}}\right) = \prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right)$$

and

$$\begin{aligned}
&\int_{[0,1]^{2d}} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\
&= \int_{[0,1]^{2d}} \prod_{j=1}^{d}\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi \mathrm{i} h(x_j-y_j)}}{|h|^{\alpha}}\right)\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\
&= \prod_{j=1}^{d}\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \left(\frac{1}{|h|^{\alpha}}\int_0^1\int_0^1 e^{2\pi \mathrm{i} h(x_j-y_j)}\,\mathrm{d}x_j\,\mathrm{d}y_j\right)\right) \\
&= \prod_{j=1}^{d}\beta_j,
\end{aligned}$$

where we have used the fact that for $x, y \in [0,1)$ and $h \neq 0$,

$$\int_0^1\int_0^1 e^{2\pi \mathrm{i} h(x-y)}\,\mathrm{d}x\,\mathrm{d}y = \int_0^1 e^{2\pi \mathrm{i} hx}\,\mathrm{d}x \int_0^1 e^{-2\pi \mathrm{i} hy}\,\mathrm{d}y = 0.$$

This completes the proof. □

The following theorem gives sufficient conditions for QMC rules to be strongly tractable in weighted Korobov spaces. We see from the theorem that the ε-exponent of strong tractability is at most 2.

Theorem 2.9 *Suppose that*

$$\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty.$$

Further, suppose for all $d \geq 1$ there exists a set of quadrature points $P_{n,d}$ such that

$$e^2_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) \leq \frac{b}{n}\prod_{j=1}^{d}(\beta_j + a\gamma_j),$$

where $a, b > 0$ are bounded independently of d. Then for all $d \geq 1$, we have

$$e_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) \leq Cn^{-\frac{1}{2}}e_{0,d}(K_{d,\beta,\gamma}),$$

with

$$C = b^{\frac{1}{2}}\prod_{j=1}^{\infty}\left(1+\frac{a\gamma_j}{\beta_j}\right)^{\frac{1}{2}} \leq b^{\frac{1}{2}}\exp\left(\frac{a}{2}\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j}\right) < \infty.$$

Proof. Recall from Lemma 2.7 that the initial error satisfies

$$e^2_{0,d}(K_{d,\beta,\gamma}) = \prod_{j=1}^{d}\beta_j.$$

We have

$$\begin{aligned} e^2_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) &\leq \frac{b}{n}\prod_{j=1}^{d}(\beta_j + a\gamma_j) \\ &= \frac{b}{n}\prod_{j=1}^{d}\left(1+\frac{a\gamma_j}{\beta_j}\right)\prod_{j=1}^{d}\beta_j \\ &\leq \frac{b}{n}\prod_{j=1}^{\infty}\left(1+\frac{a\gamma_j}{\beta_j}\right)e^2_{0,d}(K_{d,\beta,\gamma}). \end{aligned}$$

Thus $e_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) \leq Cn^{-\frac{1}{2}}e_{0,d}(K_{d,\beta,\gamma})$, where

$$C = b^{\frac{1}{2}}\prod_{j=1}^{\infty}\left(1+\frac{a\gamma_j}{\beta_j}\right)^{\frac{1}{2}} = b^{\frac{1}{2}}\exp\left(\frac{1}{2}\sum_{j=1}^{\infty}\log\left(1+\frac{a\gamma_j}{\beta_j}\right)\right).$$

Since $\log(1+x) \leq x$ for all $x > 0$ and $\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty$, we have

$$C \leq b^{\frac{1}{2}}\exp\left(\frac{1}{2}\sum_{j=1}^{\infty}\frac{a\gamma_j}{\beta_j}\right) = b^{\frac{1}{2}}\exp\left(\frac{a}{2}\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j}\right) < \infty.$$

This completes the proof. □

Clearly the QMC mean in Lemma 2.8 has an upper bound of the form

$$\frac{b}{n}\prod_{j=1}^{d}(\beta_j + a\gamma_j), \tag{2.9}$$

with $a = 2\zeta(\alpha)$ and $b = 1$. Thus the assumption on the existence of the set $P_{n,d}$ of quadrature points in Theorem 2.9 is always justified, and this holds with no assumptions on the weights. If d is small, the bound would be of interest for the unweighted case $\beta_j = \gamma_j = 1$. We remark that the condition

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty \tag{2.10}$$

is not only sufficient but is in fact necessary for strong QMC tractability in weighted Korobov spaces. It is also worth mentioning that a necessary and sufficient condition for QMC tractability in weighted Korobov spaces is

$$\limsup_{d\to\infty} \frac{\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j}}{\log d} < \infty.$$

The underlying arguments may be found in [12] and [36].

Throughout the thesis, we shall call bounds of the form (2.9) the 'strong tractability error bounds' in weighted Korobov spaces, and we will assume without further comment that the condition (2.10) holds.

2.3 Weighted Sobolev spaces

Weighted Sobolev spaces are tensor product reproducing kernel Hilbert spaces of non-periodic functions. These spaces have been considered previously in works such as [11], [12], [25], [35], and [36].

2.3.1 The 1-dimensional case

We start by defining the 1-dimensional Sobolev space which is parameterized by positive weights β and γ and a real number $a \in [0, 1]$. The Hilbert space $H_{1,\beta,\gamma}$ is the space of absolutely continuous functions whose first derivatives belong to $L_2([0,1])$. The inner product in $H_{1,\beta,\gamma}$ is defined by

$$\langle f, g\rangle_{1,\beta,\gamma} = \beta^{-1} f(a)g(a) + \gamma^{-1} \int_0^1 f'(x)g'(x)\,dx,$$

with corresponding norm given by

$$\|f\|_{1,\beta,\gamma} = \left(\beta^{-1} f(a)^2 + \gamma^{-1} \int_0^1 f'(x)^2 \, \mathrm{d}x\right)^{\frac{1}{2}}$$

Note that $\beta = 1$ and $a = 1$ are the common choices (see [12] and [36]), but a general choice of the parameter a is also considered in [25].

The expression for the reproducing kernel is given in the next lemma.

Lemma 2.10 *The reproducing kernel for the space $H_{1,\beta,\gamma}$ is*

$$K_{1,\beta,\gamma}(x,y) = \beta + \gamma\sigma_a(x,y),$$

where

$$\sigma_a(x,y) = \begin{cases} \min(|x-a|, |y-a|), & \textit{if } (x-a)(y-a) > 0, \\ 0, & \textit{if } (x-a)(y-a) \leq 0. \end{cases}$$

Proof. For $y > a$, we have

$$K_{1,\beta,\gamma}(x,y) = \begin{cases} \beta, & \text{if } 0 \leq x \leq a, \\ \beta + \gamma(x-a), & \text{if } a < x < y, \\ \beta + \gamma(y-a), & \text{if } y \leq x \leq 1, \end{cases}$$

and so

$$\frac{\partial}{\partial x} K_{1,\beta,\gamma}(x,y) = \begin{cases} \gamma, & \text{if } a < x < y, \\ 0, & \text{otherwise.} \end{cases}$$

In this case, for any $f \in H_{1,\beta,\gamma}$ we have

$$\begin{aligned} \langle f, K_{1,\beta,\gamma}(\cdot,y)\rangle_1 &= \beta^{-1} f(a) K_{1,\beta,\gamma}(a,y) + \gamma^{-1} \int_0^1 f'(x) \frac{\partial}{\partial x} K_{1,\beta,\gamma}(x,y) \, \mathrm{d}x \\ &= \beta^{-1} f(a)\beta + \gamma^{-1}\gamma \int_a^y f'(x) \, \mathrm{d}x \\ &= f(a) + [f(y) - f(a)] = f(y). \end{aligned}$$

For $y \leq a$, we have

$$K_{1,\beta,\gamma}(x,y) = \begin{cases} \beta + \gamma(a-y), & \text{if } 0 \leq x \leq y, \\ \beta + \gamma(a-x), & \text{if } y < x < a, \\ \beta, & \text{if } a \leq x \leq 1, \end{cases}$$

and so

$$\frac{\partial}{\partial x}K_{1,\beta,\gamma}(x,y) = \begin{cases} -\gamma, & \text{if } y < x < a, \\ 0, & \text{otherwise.} \end{cases}$$

In this case,

$$\begin{aligned} \langle f, K_{1,\beta,\gamma}(\cdot,y)\rangle_1 &= \beta^{-1} f(a) K_{1,\beta,\gamma}(a,y) + \gamma^{-1}\int_0^1 f'(x)\frac{\partial}{\partial x}K_{1,\beta,\gamma}(x,y)\,\mathrm{d}x \\ &= \beta^{-1} f(a)\beta + \gamma^{-1}(-\gamma)\int_y^a f'(x)\,\mathrm{d}x \\ &= f(a) - [f(a) - f(y)] = f(y). \end{aligned}$$

Thus for all $f \in H_{1,\beta,\gamma}$ and $y \in [0,1]$ we have $\langle f, K_{1,\beta,\gamma}(\cdot,y)\rangle_1 = f(y)$, which is the required property of a reproducing kernel. □

Recall that for any arbitrary kernel, there corresponds a shift-invariant kernel defined by (2.4). In the following lemma, we give the expression of the shift-invariant kernel associated with $K_{1,\beta,\gamma}$ given in Lemma 2.10.

Lemma 2.11 *The shift-invariant kernel associated with the reproducing kernel $K_{1,\beta,\gamma}$ from Lemma 2.10 is given by*

$$K^*_{1,\beta,\gamma}(x,y) = \beta + \gamma\left(|x-y|^2 - |x-y| + a^2 - a + \tfrac{1}{2}\right).$$

Proof. By definition,

$$K^*_{1,\beta,\gamma}(x,y) = \int_0^1 \left(\beta + \gamma\sigma_a(\{x+\Delta\},\{y+\Delta\})\right)\mathrm{d}\Delta = \beta + \gamma\kappa_a(x,y),$$

where

$$\kappa_a(x,y) = \int_0^1 \sigma_a(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta.$$

Let us assume without lost of generality that $x \le y$. Then there are three possible arrangements of the values of $x+\Delta$ and $y+\Delta$:

Case 1: $x+\Delta \le y+\Delta < 1$, which implies $\Delta < 1-y$.

Case 2: $x+\Delta < 1 \le y+\Delta$, which implies $1-y \le \Delta < 1-x$.

Case 3: $1 \le x+\Delta \le y+\Delta$, which implies $\Delta \ge 1-x$.

Corresponding to the three cases, we have

Case 1: $\{x+\Delta\} = x+\Delta$, $\{y+\Delta\} = y+\Delta = \{x+\Delta\} - x + y$.

Case 2: $\{x+\Delta\} = x+\Delta$, $\{y+\Delta\} = y+\Delta-1 = \{x+\Delta\} - x + y - 1$.

Case 3: $\{x+\Delta\} = x+\Delta-1$, $\{y+\Delta\} = y+\Delta-1 = \{x+\Delta\} - x + y$.

Now let $u = \{x+\Delta\}$. Then for any of the three cases above we have $\mathrm{d}u = \mathrm{d}\Delta$. Thus

$$\begin{aligned}
\kappa_a(x,y) &= \int_0^{1-y} \sigma_a(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta + \int_{1-y}^{1-x} \sigma_a(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta \\
&\quad + \int_{1-x}^{1} \sigma_a(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta \\
&= \int_x^{x+1-y} \sigma_a(u, u-x+y)\,\mathrm{d}u + \int_{x+1-y}^{1} \sigma_a(u, u-x+y-1)\,\mathrm{d}u \\
&\quad + \int_0^{x} \sigma_a(u, u-x+y)\,\mathrm{d}u \\
&= \int_0^{x-y+1} \sigma_a(u, u-x+y)\,\mathrm{d}u + \int_{x-y+1}^{1} \sigma_a(u, u-x+y-1)\,\mathrm{d}u.
\end{aligned}$$

Since $x \le y$ which leads to $u - x + y \ge u$, it follows from the definition of σ_a in Lemma 2.10 that when $0 \le u \le x - y + 1$ we have

$$\sigma_a(u, u-x+y) = \begin{cases} u - a, & \text{if } u > a, \\ -u + x - y + a, & \text{if } u < x - y + a, \\ 0, & \text{otherwise.} \end{cases}$$

Similarly, for $x - y + 1 < u \le 1$ we have

$$\sigma_a(u, u-x+y-1) = \begin{cases} u - x + y - 1 - a, & \text{if } u > x - y + 1 + a, \\ -u + a, & \text{if } u < a, \\ 0, & \text{otherwise.} \end{cases}$$

Now we could have $x - y + a > 0$ in which case we have $x - y + 1 + a > 1$. Alternatively, if $x - y + a \le 0$, then $x - y + 1 + a \le 1$. In either of these two situations, the value of a could either satisfy $a \le x - y + 1$ or satisfy $a > x - y + 1$. Hence there are four possibilities:

Possibility 1: When $0 < x - y + a \le a \le x - y + 1 \le 1$, we have

$$\sigma_a(u, u-x+y) = \begin{cases} -u + x - y + a, & \text{if } 0 \le u < x - y + a, \\ 0, & \text{if } x - y + a \le u \le a, \\ u - a, & \text{if } a < u \le x - y + 1, \end{cases}$$

and

$$\sigma_a(u, u-x+y-1) = 0 \text{ for } x-y+1 < u \le 1.$$

It then follows that

$$\begin{aligned} \kappa_a(x,y) &= \int_0^{x-y+a} (-u+x-y+a)\,\mathrm{d}u + \int_a^{x-y+1} (u-a)\,\mathrm{d}u \\ &= (x-y)^2 + (x-y) + a^2 - a + \tfrac{1}{2}. \end{aligned}$$

Possibility 2: When $0 < x-y+a \le x-y+1 < a \le 1$, we can obtain expressions for $\sigma_a(u, u-x+y)$ and $\sigma_a(u, u-x+y-1)$ as above and thus obtain

$$\begin{aligned} \kappa_a(x,y) &= \int_0^{x-y+a} (-u+x-y+a)\,\mathrm{d}u + \int_{x-y+1}^{a} (-u+a)\,\mathrm{d}u \\ &= (x-y)^2 + (x-y) + a^2 - a + \tfrac{1}{2}. \end{aligned}$$

Possibility 3: When $0 \le a \le x-y+1 \le x-y+1+a \le 1$, we obtain

$$\begin{aligned} \kappa_a(x,y) &= \int_a^{x-y+1} (u-a)\,\mathrm{d}u + \int_{x-y+1+a}^{1} (u-x+y-1-a)\,\mathrm{d}u \\ &= (x-y)^2 + (x-y) + a^2 - a + \tfrac{1}{2}. \end{aligned}$$

Possibility 4: When $0 \le x-y+1 \le a < x-y+1+a \le 1$, we obtain

$$\begin{aligned} \kappa_a(x,y) &= \int_{x-y+1}^{a} (-u+a)\,\mathrm{d}u + \int_{x-y+1+a}^{1} (u-x+y-1-a)\,\mathrm{d}u \\ &= (x-y)^2 + (x-y) + a^2 - a + \tfrac{1}{2}. \end{aligned}$$

Since the results are the same for all four possibilities, we have for $x \le y$,

$$\kappa_a(x,y) = (x-y)^2 + (x-y) + a^2 - a + \tfrac{1}{2}.$$

By symmetry, for $x > y$ we have

$$\kappa_a(x,y) = (y-x)^2 + (y-x) + a^2 - a + \tfrac{1}{2}.$$

Thus

$$\kappa_a(x,y) = |x-y|^2 - |x-y| + a^2 - a + \tfrac{1}{2},$$

and hence

$$K^*_{1,\beta,\gamma}(x,y) = \beta + \gamma\left(|x-y|^2 - |x-y| + a^2 - a + \tfrac{1}{2}\right),$$

which completes the proof. □

2.3.2 The d-dimensional case

Now we define our d-dimensional weighted Sobolev space parameterized by a real vector $\boldsymbol{a} \in [0,1]^d$. Suppose we have two positive sequences $\boldsymbol{\beta} = \{\beta_j\}$ and $\boldsymbol{\gamma} = \{\gamma_j\}$ satisfying

$$\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots .$$

Similar to the d-dimensional weighted Korobov spaces, we define the d-dimensional weighted Sobolev space $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ as the tensor product

$$H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} := H^{(1)}_{1,\beta_1,\gamma_1} \otimes H^{(2)}_{1,\beta_2,\gamma_2} \otimes \cdots \otimes H^{(d)}_{1,\beta_d,\gamma_d}$$

of d different 1-dimensional weighted Sobolev spaces with different weights.

For $f(\boldsymbol{x}) = \prod_{j=1}^{d} f_j(x_j)$ and $g(\boldsymbol{x}) = \prod_{j=1}^{d} g_j(x_j)$ with $f_j, g_j \in H^{(j)}_{1,\beta_j,\gamma_j}$, again we define their inner product in $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ as in Lemma 2.1 by $\langle f, g\rangle_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} := \prod_{j=1}^{d} \langle f_j, g_j\rangle^{(j)}_{1,\beta_j,\gamma_j}$. From this it can be verified that the inner product for any general $f, g \in H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is given by

$$\langle f, g\rangle_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} = \sum_{\mathrm{u}\subseteq\mathcal{D}} \left(\prod_{j\notin \mathrm{u}} \beta_j^{-1} \prod_{j\in\mathrm{u}} \gamma_j^{-1} \int_{[0,1]^{|\mathrm{u}|}} \frac{\partial^{|\mathrm{u}|}}{\partial \boldsymbol{x}_{\mathrm{u}}} f(\boldsymbol{x}_{\mathrm{u}}, \boldsymbol{a}) \frac{\partial^{|\mathrm{u}|}}{\partial \boldsymbol{x}_{\mathrm{u}}} g(\boldsymbol{x}_{\mathrm{u}}, \boldsymbol{a}) \, \mathrm{d}\boldsymbol{x}_{\mathrm{u}} \right),$$

where $\mathcal{D} = \{1, 2, \ldots, d\}$, $(\boldsymbol{x}_{\mathrm{u}}, \boldsymbol{a})$ is a d-dimensional vector whose j-th component is x_j if $j \in \mathrm{u}$ and a_j if $j \notin \mathrm{u}$, and $\mathrm{d}\boldsymbol{x}_{\mathrm{u}} = \prod_{j\in\mathrm{u}} \mathrm{d}x_j$. The norm in $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is

$$\|f\|_{d,\boldsymbol{\beta},\boldsymbol{\gamma}} = \left[\sum_{\mathrm{u}\subseteq\mathcal{D}} \left(\prod_{j\notin \mathrm{u}} \beta_j^{-1} \prod_{j\in\mathrm{u}} \gamma_j^{-1} \int_{[0,1]^{|\mathrm{u}|}} \left(\frac{\partial^{|\mathrm{u}|}}{\partial \boldsymbol{x}_{\mathrm{u}}} f(\boldsymbol{x}_{\mathrm{u}}, \boldsymbol{a}) \right)^2 \mathrm{d}\boldsymbol{x}_{\mathrm{u}} \right) \right]^{\frac{1}{2}}$$

It follows from Lemma 2.1 that the reproducing kernel for $H_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is

$$K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) = \prod_{j=1}^{d} K_{1,\beta_j,\gamma_j}(x_j, y_j) = \prod_{j=1}^{d} \left(\beta_j + \gamma_j \sigma_{a_j}(x_j, y_j)\right), \tag{2.11}$$

where $\sigma_{a_j}(x_j, y_j)$ is as given in Lemma 2.10, and the shift-invariant kernel $K^*_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ associated with $K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is given by

$$\begin{aligned} K^*_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) &= \prod_{j=1}^{d} K^*_{1,\beta_j,\gamma_j}(x_j, y_j) \\ &= \prod_{j=1}^{d} \left[\beta_j + \gamma_j \left(|x_j - y_j|^2 - |x_j - y_j| + a_j^2 - a_j + \tfrac{1}{2}\right)\right]. \end{aligned} \tag{2.12}$$

In the following lemma, we show that $K^*_{d,\beta,\gamma}$ is a kernel for a weighted Korobov space (cf. (2.7)) with $\alpha = 2$.

Lemma 2.12 *The kernel* $K^*_{d,\beta,\gamma}$ *of* (2.12) *may be written as*

$$K^*_{d,\beta,\gamma}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d}\left(\hat{\beta}_j + \hat{\gamma}_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_j-y_j)}}{h^2}\right),$$

where

$$\hat{\beta}_j = \beta_j + \gamma_j\left(a_j^2 - a_j + \frac{1}{3}\right) \quad \textit{and} \quad \hat{\gamma}_j = \frac{\gamma_j}{2\pi^2}.$$

Proof. We have from Lemma 2.11 that

$$\begin{aligned} K^*_{1,\beta,\gamma}(x,y) &= \beta + \gamma\left(|x-y|^2 - |x-y| + a^2 - a + \tfrac{1}{2}\right) \\ &= \beta + \gamma\left(B_2(|x-y|) + a^2 - a + \tfrac{1}{3}\right), \end{aligned}$$

where B_2 is the Bernoulli polynomial given by $B_2(x) = x^2 - x + \frac{1}{6}$, and can be written as the Fourier expansion in (2.8) with $\alpha = 2$. It then follows that we can write $K^*_{1,\beta,\gamma}$ as

$$\begin{aligned} K^*_{1,\beta,\gamma}(x,y) &= \beta + \gamma\left(\frac{1}{2\pi^2}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h|x-y|}}{h^2} + a^2 - a + \frac{1}{3}\right) \\ &= \beta + \gamma\left(a^2 - a + \frac{1}{3}\right) + \frac{\gamma}{2\pi^2}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h|x-y|}}{h^2}. \end{aligned}$$

Hence

$$\begin{aligned} K^*_{d,\beta,\gamma}(\boldsymbol{x},\boldsymbol{y}) &= \prod_{j=1}^{d} K^*_{1,\beta_j,\gamma_j}(x_j,y_j) \\ &= \prod_{j=1}^{d}\left[\beta_j + \gamma_j\left(a_j^2 - a_j + \frac{1}{3}\right) + \frac{\gamma_j}{2\pi^2}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h|x_j-y_j|}}{h^2}\right]. \end{aligned}$$

Since

$$\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_j-y_j)}}{h^2} = \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(y_j-x_j)}}{h^2},$$

this completes the proof. □

2.3.3 QMC rules in weighted Sobolev spaces

We give the expressions for the errors of QMC rules in weighted Sobolev spaces in the following lemma.

Lemma 2.13 *We have*

$$e_{0,d}^2(K_{d,\beta,\gamma}) = \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left(a_j^2 - a_j + \tfrac{1}{3}\right)\right)$$

and

$$\begin{aligned} & e_{n,d}^2(P_{n,d}, K_{d,\beta,\gamma}) \\ = & \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left(a_j^2 - a_j + \tfrac{1}{3}\right)\right) - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \varrho_{a_j}(x_{i,j})\right) \\ & + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \sigma_{a_j}(x_{i,j}, x_{k,j})\right), \end{aligned}$$

where σ_{a_j} is as given in Lemma 2.10 and

$$\varrho_a(x) = \begin{cases} (x-a)\left(1 - \frac{a}{2} - \frac{x}{2}\right), & \text{if } x > a, \\ (a-x)\left(\frac{a}{2} + \frac{x}{2}\right), & \text{if } x \le a. \end{cases}$$

Proof. We have from Lemma 2.2 that

$$e_{0,d}^2(K_{d,\beta,\gamma}) = \int_{[0,1]^{2d}} K_{d,\beta,\gamma}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y}$$

and

$$\begin{aligned} e_{n,d}^2(P_{n,d}, K_{d,\beta,\gamma}) = & \int_{[0,1]^{2d}} K_{d,\beta,\gamma}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} - \frac{2}{n} \sum_{i=0}^{n-1} \int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x}_i, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \\ & + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} K_{d,\beta,\gamma}(\boldsymbol{x}_i, \boldsymbol{x}_k). \end{aligned}$$

Thus, to obtain the expressions for these errors, we need to obtain

$$\int_{[0,1]^d} K_{d,\beta,\gamma}(\boldsymbol{x}_i, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \quad \text{and} \quad \int_{[0,1]^{2d}} K_{d,\beta,\gamma}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y}.$$

For $x > a$, we have

$$K_{1,\beta,\gamma}(x, y) = \begin{cases} \beta, & \text{if } 0 \le y \le a, \\ \beta + \gamma(y - a), & \text{if } a < y < x, \\ \beta + \gamma(x - a), & \text{if } x \le y \le 1, \end{cases}$$

and so

$$\begin{aligned}
&\int_0^1 K_{1,\beta,\gamma}(x,y)\,\mathrm{d}y \\
&= \int_0^a \beta\,\mathrm{d}x + \int_a^x [\beta + \gamma(y-a)]\,\mathrm{d}y + \int_x^1 [\beta + \gamma(x-a)]\,\mathrm{d}y \\
&= \beta + \gamma(x-a)\left(1 - \frac{a}{2} - \frac{x}{2}\right).
\end{aligned}$$

For $x \le a$, we have

$$K_{1,\beta,\gamma}(x,y) = \begin{cases} \beta + \gamma(a-x), & \text{if } 0 \le y \le x, \\ \beta + \gamma(a-y), & \text{if } x < y < a, \\ \beta, & \text{if } a \le y \le 1, \end{cases}$$

and so

$$\begin{aligned}
&\int_0^1 K_{1,\beta,\gamma}(x,y)\,\mathrm{d}y \\
&= \int_0^x [\beta + \gamma(a-x)]\,\mathrm{d}y + \int_x^a [\beta + \gamma(a-y)]\,\mathrm{d}y + \int_a^1 \beta\,\mathrm{d}y \\
&= \beta + \gamma(a-x)\left(\frac{a}{2} + \frac{x}{2}\right).
\end{aligned}$$

Thus we have

$$\int_0^1 K_{1,\beta,\gamma}(x,y)\,\mathrm{d}y = \beta + \gamma\varrho_a(x),$$

and hence the first integral is

$$\int_{[0,1]^d} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x}_i,\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \prod_{j=1}^d \int_0^1 K_{1,\beta_j,\gamma_j}(x_{i,j},y_j)\,\mathrm{d}y_j = \prod_{j=1}^d \left(\beta_j + \gamma_j\varrho_{a_j}(x_{i,j})\right).$$

Now we obtain the second integral. It can be shown that

$$\int_0^1 \varrho_a(x)\,\mathrm{d}x = a^2 - a + \tfrac{1}{3},$$

and so

$$\int_0^1\int_0^1 K_{1,\beta,\gamma}(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_0^1 (\beta + \gamma\varrho_a(x))\,\mathrm{d}x = \beta + \gamma\left(a^2 - a + \tfrac{1}{3}\right),$$

and this leads to

$$\begin{aligned}
\int_{[0,1]^{2d}} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} &= \prod_{j=1}^d \int_0^1\int_0^1 K_{1,\beta_j,\gamma_j}(x_j,y_j)\,\mathrm{d}x_j\,\mathrm{d}y_j \\
&= \prod_{j=1}^d \left(\beta_j + \gamma_j\left(a_j^2 - a_j + \tfrac{1}{3}\right)\right).
\end{aligned}$$

This completes the proof. □

We remark that when all the β_j are 1 and all of the components of $\boldsymbol{a}$ are also 1, $e_{n,d}(P_{n,d}, K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}})$ in Lemma 2.16 is simply the weighted version of the L_2 star discrepancy considered in earlier work such as [9] and [35]. When all the β_j are 1 and all of the components of $\boldsymbol{a}$ are $\frac{1}{2}$, then $e_{n,d}(P_{n,d}, K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}})$ is the weighted version of the L_2 centered discrepancy discussed in [8].

The expression for the QMC mean $E_{n,d}(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}})$ in weighted Sobolev spaces is given in the next lemma.

Lemma 2.14 *We have*

$$E_{n,d}\left(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}\right) = \frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(a_j^2 - a_j + \tfrac{1}{2}\right)\right) - \prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(a_j^2 - a_j + \tfrac{1}{3}\right)\right)\right).$$

Proof. It follows from Lemma 2.5 that

$$E_{n,d}(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}) = \frac{1}{n}\left(\int_{[0,1]^d} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \int_{[0,1]^{2d}} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right),$$

where $K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is as given in (2.11).

We have from the definition of $K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ that

$$\begin{aligned}
\int_{[0,1]^d} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} &= \int_{[0,1]^d}\left(\prod_{j=1}^{d}(\beta_j + \gamma_j|x_j - a_j|)\right)\mathrm{d}\boldsymbol{x} \\
&= \prod_{j=1}^{d}\left(\beta_j + \gamma_j\int_0^1 |x_j - a_j|\,\mathrm{d}x_j\right) \\
&= \prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(a_j^2 - a_j + \tfrac{1}{2}\right)\right),
\end{aligned}$$

since

$$\int_0^1 |x_j - a_j|\,\mathrm{d}x_j = \int_0^{a_j}(a_j - x_j)\,\mathrm{d}x_j + \int_{a_j}^1 (x_j - a_j)\,\mathrm{d}x_j = a_j^2 - a_j + \tfrac{1}{2}.$$

Also, we see from the proof of Lemma 2.13 that

$$\int_{[0,1]^{2d}} K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} = \prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(a_j^2 - a_j + \tfrac{1}{3}\right)\right).$$

This completes the proof. □

Theorem 2.15 below gives sufficient conditions for QMC rules to be strongly tractable in weighted Sobolev spaces, with the ε-exponent of strong tractability being at most 2. Note that Theorem 2.15 is very similar to Theorem 2.9 for weighted Korobov spaces.

Theorem 2.15 *Suppose that*

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty.$$

Further, suppose for all $d \geq 1$ there exists a set of quadrature points $P_{n,d}$ such that

$$e_{n,d}^2(P_{n,d}, K_{d,\beta,\gamma}) \leq \frac{b}{n} \prod_{j=1}^{d} (\beta_j + a\gamma_j),$$

where $a \geq \frac{1}{12}$ and $b > 0$ are bounded independently of d. Then for all $d \geq 1$, we have

$$e_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) \leq C n^{-\frac{1}{2}} e_{0,d}(K_{d,\beta,\gamma}),$$

with

$$C = b^{\frac{1}{2}} \prod_{j=1}^{\infty} \left(1 + \frac{(12a-1)\gamma_j}{12\beta_j}\right)^{\frac{1}{2}} \leq b^{\frac{1}{2}} \exp\left(\frac{12a-1}{24} \sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j}\right) < \infty.$$

Proof. Recall from Lemma 2.13 that the initial worst-case error satisfies

$$e_{0,d}^2(K_{d,\beta,\gamma}) = \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left(a_j^2 - a_j + \tfrac{1}{3}\right)\right).$$

We have

$$\begin{aligned}
& e_{n,d}^2(P_{n,d}, K_{d,\beta,\gamma}) \\
\leq\ & \frac{b}{n} \prod_{j=1}^{d} (\beta_j + a\gamma_j) \\
=\ & \frac{b}{n} \prod_{j=1}^{d} \left(\frac{\beta_j + a\gamma_j}{\beta_j + \gamma_j \left(a_j^2 - a_j + \frac{1}{3}\right)}\right) \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left(a_j^2 - a_j + \tfrac{1}{3}\right)\right) \\
\leq\ & \frac{b}{n} \prod_{j=1}^{d} \left(\frac{\beta_j + a\gamma_j}{\beta_j + \frac{\gamma_j}{12}}\right) e_{0,d}^2(K_{d,\beta,\gamma}) \\
=\ & \frac{b}{n} \prod_{j=1}^{d} \left(1 + \frac{(12a-1)\gamma_j}{12\beta_j + \gamma_j}\right) e_{0,d}^2(K_{d,\beta,\gamma}) \\
\leq\ & \frac{b}{n} \prod_{j=1}^{\infty} \left(1 + \frac{(12a-1)\gamma_j}{12\beta_j}\right) e_{0,d}^2(K_{d,\beta,\gamma}).
\end{aligned}$$

Thus $e_{n,d}(P_{n,d}, K_{d,\beta,\gamma}) \leq C n^{-\frac{1}{2}} e_{0,d}(K_{d,\beta,\gamma})$, where

$$C = b^{\frac{1}{2}} \prod_{j=1}^{\infty} \left(1 + \frac{(12a-1)\gamma_j}{12\beta_j}\right)^{\frac{1}{2}} = b^{\frac{1}{2}} \exp\left(\frac{1}{2} \sum_{j=1}^{\infty} \log\left(1 + \frac{(12a-1)\gamma_j}{12\beta_j}\right)\right).$$

Since $\log(1+x) \leq x$ for all $x > 0$ and $\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty$, we have

$$C \leq b^{\frac{1}{2}} \exp\left(\frac{1}{2}\sum_{j=1}^{\infty} \frac{(12a-1)\gamma_j}{12\beta_j}\right) = b^{\frac{1}{2}} \exp\left(\frac{12a-1}{24}\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j}\right) < \infty.$$

This completes the proof. □

Similar to the weighted Korobov spaces, the assumption on the existence of the set $P_{n,d}$ of quadrature points in Theorem 2.15 is always justified as the QMC mean in Lemma 2.14 has an upper bound of the form

$$\frac{b}{n}\prod_{j=1}^{d}(\beta_j + a\gamma_j), \tag{2.13}$$

with $a = \frac{1}{2}$ and $b = 1$. If d is small, this bound would be of interest for the unweighted case $\beta_j = \gamma_j = 1$. We remark that the condition

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty \tag{2.14}$$

is necessary and sufficient for strong QMC tractability in weighted Sobolev spaces. Although we are mainly concerned with strong QMC tractability, we remark that QMC tractability in weighted Sobolev spaces holds if and only if

$$\limsup_{d\to\infty} \frac{\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j}}{\log d} < \infty.$$

The underlying arguments can be found in [12], [25], and [35]. Again throughout the thesis, we shall call bounds of the form (2.13) the 'strong tractability error bounds' in weighted Sobolev spaces, and we will assume without further comment that the condition (2.14) holds.

For simplicity, we will take $\boldsymbol{a} = \mathbf{1}$ in the rest of the thesis. In this case, the reproducing kernel is

$$K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d}\left(\beta_j + \gamma_j[1 - \max(x_j, y_j)]\right).$$

The expressions for the errors and the QMC mean for $\boldsymbol{a} = \mathbf{1}$ are given in the next two lemmas.

Lemma 2.16 *For $\boldsymbol{a} = \mathbf{1}$, we have*

$$e_{0,d}^2(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}) = \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{3}\right)$$

and

$$\begin{aligned} e_{n,d}^2(P_{n,d}, K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}) &= \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{3}\right) - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{d} \left[\beta_j + \frac{\gamma_j}{2}\left(1 - x_{i,j}^2\right)\right] \\ &+ \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[1 - \max(x_{i,j}, x_{k,j})\right]\right). \end{aligned}$$

Lemma 2.17 *For $\boldsymbol{a} = \mathbf{1}$, we have*

$$E_{n,d}\left(K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}\right) = \frac{1}{n} \left(\prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{2}\right) - \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{3}\right) \right).$$

Chapter 3

Constructing Rank-1 Lattice Rules in Weighted Korobov Spaces

Theorem 2.9 gives sufficient conditions for a family of QMC rules to be strongly tractable in weighted Korobov spaces: the sum of γ_j/β_j is finite, and there must exist a rule in the family with square worst-case error bounded by an expression of a certain form. In this chapter, we show by using an averaging argument that when the number of points n is a prime number, there exists a rank-1 lattice rule with square worst-case error bounded by an expression of this desired form. We also show by using another averaging argument that the generating vector of such a rule can be constructed by a component-by-component algorithm.

An unweighted version (when all the weights β_j and γ_j are taken to be 1) of some results from this chapter was given in [33].

3.1 The existence of good rules

Weighted Korobov spaces are tensor product reproducing kernel Hilbert spaces of periodic functions. We recall from Chapter 2 that these spaces are parameterized by a real parameter $\alpha > 1$, which is taken to be an even integer in practice, and two sequences of positive weights $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ satisfying

$$\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots .$$

Now we recall from (1.4) that rank-1 lattice rules are QMC rules with quadrature points given by the set

$$\left\{ \left\{ \frac{i\boldsymbol{z}}{n} \right\} : i = 0, \ldots, n-1 \right\},$$

where $\boldsymbol{z} \in \mathcal{Z}_n^d$ is the 'generating vector' with $\mathcal{Z}_n$ given by (1.5). In this section, we first give the explicit expression for the square worst-case error and give the expression for the mean square worst-case error when n is prime. We then derive several upper bounds on the mean and thus prove the existence of rank-1 lattice rules that achieve strong tractability error bounds (see Theorem 2.9) in weighted Korobov spaces.

3.1.1 Square worst-case error

Let $e_{n,d}(\boldsymbol{z})$ denote the worst-case error of a rank-1 lattice rule with generating vector $\boldsymbol{z}$ in weighted Korobov spaces. The expression for $e_{n,d}^2(\boldsymbol{z})$ is given in the following lemma.

Lemma 3.1 *We have*

$$e_{n,d}^2(\boldsymbol{z}) = -\prod_{j=1}^{d} \beta_j + \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z_j / n}}{|h|^\alpha} \right).$$

Proof. It follows from Lemma 2.7 with $\boldsymbol{x}_i = \left\{ \frac{i\boldsymbol{z}}{n} \right\}$ that

$$e_{n,d}^2(\boldsymbol{z}) = -\prod_{j=1}^{d} \beta_j + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h (i-k) z_j / n}}{|h|^\alpha} \right).$$

The result now follows from the fact that as i and k go from 0 to $n-1$, the values of $(i-k) \bmod n$ are just $0, \ldots, n-1$ in some order, with each value occurring n times. $\square$

As mentioned earlier, in practice, we take $\alpha \geq 2$ to be an even integer so that the infinite sum in the last term of $e_{n,d}^2(\boldsymbol{z})$ can be written in terms of the Bernoulli polynomials, and thus allow $e_{n,d}^2(\boldsymbol{z})$ to be calculated in $O(nd)$ operations.

3.1.2 Mean and upper bound when n is prime

We define the mean square worst-case error over all values of $\boldsymbol{z} \in \mathcal{Z}_n^d$ by

$$M_{n,d} := \frac{1}{[\phi(n)]^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} e_{n,d}^2(\boldsymbol{z}).$$

For simplicity in this chapter, we will restrict n to be a prime number. In this case, the vector $\boldsymbol{z}$ can be chosen from $\mathbb{Z}_n^d$ with $\mathbb{Z}_n = \{1, 2, \ldots, n-1\}$. Since there are $\phi(n) = n-1$ elements in the set $\mathbb{Z}_n$, we have $(n-1)^d$ possibilities for the vector $\boldsymbol{z}$.

The explicit expression for $M_{n,d}$ when n is a prime number is given in Theorem 3.3 below. The proof of Theorem 3.3 rests upon the following useful result, which we will also use in later chapters.

Lemma 3.2 *For $\alpha > 1$, $k \in \mathbb{Z}$ and n a prime number, we define $T_\alpha(k, n)$ by*

$$T_\alpha(k,n) := \frac{1}{n-1} \sum_{z=1}^{n-1} {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i hkz/n}}{|h|^\alpha}.$$

Then

$$T_\alpha(k,n) = \begin{cases} 2\zeta(\alpha), & \textit{if } k \textit{ is a multiple of } n, \\ -\dfrac{2\zeta(\alpha)(1-n^{1-\alpha})}{n-1}, & \textit{otherwise}. \end{cases}$$

Proof. Clearly if k is a multiple of n, we have

$$T_\alpha(k,n) = \frac{1}{n-1} \sum_{z=1}^{n-1} {\sum_{h=-\infty}^{\infty}}' \frac{1}{|h|^\alpha} = 2\zeta(\alpha).$$

Now for k not a multiple of n, if h is a multiple of n, then

$$\frac{1}{n-1} \sum_{z=1}^{n-1} e^{2\pi i hkz/n} = 1,$$

and if h is not a multiple of n, then

$$\frac{1}{n-1}\sum_{z=1}^{n-1} e^{2\pi i hkz/n} = \frac{1}{n-1}\left(\sum_{z=0}^{n-1}\left(e^{2\pi i hk/n}\right)^z - 1\right) = -\frac{1}{n-1}.$$

Thus for k not a multiple of n, we have

$$\begin{aligned} T_\alpha(k,n) &= \sum_{h\equiv 0 \,(\bmod\, n)}{}' \frac{1}{|h|^\alpha} - \frac{1}{n-1}\sum_{h\not\equiv 0\,(\bmod\, n)}{}' \frac{1}{|h|^\alpha} \\ &= \sum_{m=-\infty}^{\infty}{}' \frac{1}{|mn|^\alpha} - \frac{1}{n-1}\left(\sum_{h=-\infty}^{\infty}{}' \frac{1}{|h|^\alpha} - \sum_{m=-\infty}^{\infty}{}' \frac{1}{|mn|^\alpha}\right) \\ &= \frac{2\zeta(\alpha)}{n^\alpha} - \frac{1}{n-1}\left(2\zeta(\alpha) - \frac{2\zeta(\alpha)}{n^\alpha}\right) \\ &= -2\zeta(\alpha)\left(-\frac{1}{n^\alpha} + \frac{1}{n-1} - \frac{1}{(n-1)n^\alpha}\right) \\ &= -\frac{2\zeta(\alpha)(1-n^{1-\alpha})}{n-1}. \end{aligned}$$

This completes the proof. □

Now we give the expression for $M_{n,d}$ when n is a prime number.

Theorem 3.3 *Let n be a prime number. Then*

$$M_{n,d} = -\prod_{j=1}^d \beta_j + \frac{1}{n}\prod_{j=1}^d \left(\beta_j + 2\gamma_j\zeta(\alpha)\right) + \frac{n-1}{n}\prod_{j=1}^d\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right).$$

Proof. It follows from the definition of $M_{n,d}$ and Lemma 3.1 that

$$\begin{aligned} M_{n,d} &= \frac{1}{(n-1)^d}\sum_{z\in\mathbb{Z}_n^d}\left[-\prod_{j=1}^d \beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^d\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i hkz_j/n}}{|h|^\alpha}\right)\right] \\ &= -\prod_{j=1}^d \beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^d\left(\beta_j + \gamma_j T_\alpha(k,n)\right), \end{aligned}$$

where $T_\alpha(k,n)$ is as given in Lemma 3.2. Upon separating the $k=0$ and $k\neq 0$ terms and using Lemma 3.2, the result is obtained. □

Here we obtain an upper bound on $M_{n,d}$ when n is prime. Note that this result requires a restriction on n.

Theorem 3.4 *Let n be a prime number such that $n \geq 1 + \frac{\gamma_1}{\beta_1}\zeta(\alpha)$. Then*

$$M_{n,d} \leq \frac{1}{n}\prod_{j=1}^d\left(\beta_j + 2\gamma_j\zeta(\alpha)\right).$$

Proof. For all $j \geq 1$,

$$\beta_j \geq \beta_j - \frac{2\gamma_j \zeta(\alpha)(1-n^{1-\alpha})}{n-1} \geq \beta_j - \frac{2\gamma_j\zeta(\alpha)}{n-1}.$$

Now since $\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots$, we have from the condition $n \geq 1 + \frac{\gamma_1}{\beta_1}\zeta(\alpha)$ that for all $j \geq 1$,

$$n \geq 1 + \frac{\gamma_j}{\beta_j}\zeta(\alpha),$$

which leads to

$$\beta_j - \frac{2\gamma_j\zeta(\alpha)}{n-1} \geq -\beta_j.$$

Thus we have for all $j \geq 1$,

$$\left| \beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1} \right| \leq \beta_j,$$

and so

$$\prod_{j=1}^{d} \left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1} \right) \leq \prod_{j=1}^{d} \beta_j.$$

Substituting this back into the expression for $M_{n,d}$ in Theorem 3.3, we see that

$$\begin{aligned} M_{n,d} &\leq -\prod_{j=1}^{d} \beta_j + \frac{1}{n}\prod_{j=1}^{d} (\beta_j + 2\gamma_j\zeta(\alpha)) + \frac{n-1}{n}\prod_{j=1}^{d}\beta_j \\ &\leq \frac{1}{n}\prod_{j=1}^{d} (\beta_j + 2\gamma_j\zeta(\alpha)). \end{aligned}$$

This completes the proof. □

We can obtain a slightly worse bound on $M_{n,d}$ that requires no restriction on n (except n be prime) by making use of Lemma 3.5 below. We will make use of this lemma many times in the later chapters.

Lemma 3.5 *Let $\mathcal{D} = \{1, 2, \ldots, d\}$. We have for all $a_j, b_j \in \mathbb{R}$,*

$$\prod_{j=1}^{d}(b_j + a_j) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \notin \mathfrak{u}} b_j \prod_{j \in \mathfrak{u}} a_j \right) = \prod_{j=1}^{d} b_j + \sum_{\emptyset \neq \mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \notin \mathfrak{u}} b_j \prod_{j \in \mathfrak{u}} a_j \right).$$

Proof. This result is a trivial generalization of the binomial expansion. □

Theorem 3.6 *Let n be a prime number. Then*

$$M_{n,d} \leq \min\left(\frac{2}{n}\prod_{j=1}^{d}(\beta_j + 2\gamma_j\zeta(\alpha)), \frac{1}{n}\prod_{j=1}^{d}(\beta_j + 4\gamma_j\zeta(\alpha)) \right).$$

Proof. Since

$$\begin{aligned}\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right) &\le \prod_{j=1}^{d}\left|\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right| \\ &\le \prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right) \\ &\le \prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{n-1}\right),\end{aligned}$$

we have from Theorem 3.3 that

$$M_{n,d} \le -\prod_{j=1}^{d}\beta_j + \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) + \frac{n-1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{n-1}\right). \quad (3.1)$$

Using Lemma 3.5, we can write

$$\begin{aligned}&\frac{n-1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{n-1}\right) \\ &= \frac{n-1}{n}\left(\prod_{j=1}^{d}\beta_j + \sum_{\emptyset\neq \mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(\frac{2\gamma_j\zeta(\alpha)}{n-1}\right)\right]\right) \\ &= \frac{n-1}{n}\prod_{j=1}^{d}\beta_j + \frac{n-1}{n}\sum_{\emptyset\neq \mathfrak{u}\subseteq\mathcal{D}}\left[\left(\frac{1}{n-1}\right)^{|\mathfrak{u}|}\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right] \\ &= \frac{n-1}{n}\prod_{j=1}^{d}\beta_j + \frac{1}{n}\sum_{\emptyset\neq \mathfrak{u}\subseteq\mathcal{D}}\left[\left(\frac{1}{n-1}\right)^{|\mathfrak{u}|-1}\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right].\end{aligned}$$

For $1 \le |\mathfrak{u}| \le d$,

$$\left(\frac{1}{n-1}\right)^{|\mathfrak{u}|-1} \le 1.$$

Thus

$$\begin{aligned}&\frac{n-1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{n-1}\right) \\ &\le \frac{n-1}{n}\prod_{j=1}^{d}\beta_j + \frac{1}{n}\sum_{\emptyset\neq \mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right] \\ &= \frac{n-2}{n}\prod_{j=1}^{d}\beta_j + \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right),\end{aligned}$$

and putting this into (3.1) leads to

$$M_{n,d} \le \frac{2}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) - \frac{2}{n}\prod_{j=1}^{d}\beta_j \le \frac{2}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right).$$

Also

$$\begin{aligned}
\frac{2}{n}\prod_{j=1}^{d}(\beta_j + 2\gamma_j\zeta(\alpha)) - \frac{2}{n}\prod_{j=1}^{d}\beta_j &= \frac{2}{n}\sum_{\emptyset\neq \mathrm{u}\subseteq\mathcal{D}}\left[\prod_{j\notin \mathrm{u}}\beta_j\prod_{j\in \mathrm{u}}(2\gamma_j\zeta(\alpha))\right] \\
&\leq \frac{1}{n}\sum_{\emptyset\neq \mathrm{u}\subseteq\mathcal{D}}\left[\prod_{j\notin \mathrm{u}}\beta_j\prod_{j\in \mathrm{u}}(4\gamma_j\zeta(\alpha))\right] \\
&= \frac{1}{n}\left(\prod_{j=1}^{d}(\beta_j + 4\gamma_j\zeta(\alpha)) - \prod_{j=1}^{d}\beta_j\right) \\
&\leq \frac{1}{n}\prod_{j=1}^{d}(\beta_j + 4\gamma_j\zeta(\alpha)).
\end{aligned}$$

This completes the proof. □

Clearly there must exist at least one vector $\boldsymbol{z}$ such that the square worst-case error $e^2_{n,d}(\boldsymbol{z})$ is as good as the mean $M_{n,d}$. We thus derive the following corollary.

Corollary 3.7 *Let n be a prime number. Then there exists a choice of $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that*

$$e^2_{n,d}(\boldsymbol{z}) \leq \min\left(\frac{2}{n}\prod_{j=1}^{d}(\beta_j + 2\gamma_j\zeta(\alpha)), \frac{1}{n}\prod_{j=1}^{d}(\beta_j + 4\gamma_j\zeta(\alpha))\right).$$

It is obvious that both bounds in Corollary 3.7 are of the form given in Theorem 2.9 (with $a = 2\zeta(\alpha), b = 2$ or $a = 4\zeta(\alpha), b = 1$). We thus conclude that *the family of rank-1 lattice rules with a prime number of points is strongly tractable in weighted Korobov spaces if and only if*

$$\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty.$$

3.2 Component-by-component construction

When n is a prime number, we know from the previous section that there exists a rank-1 lattice rule that achieves strong tractability error bounds in weighted Korobov spaces. In this section we prove that the generating vector of such a rule can be constructed component-by-component.

Let $e_{n,d}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1})$ denote the worst-case error for a QMC rule with the set of points $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}\}$, and let $e_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$ denote the worst-case error for a QMC rule with the set of points

$$\left\{ \left(\boldsymbol{x}_i, \left\{ \frac{i z_{d+1}}{n} \right\} \right) : 0 \leq i \leq n-1 \right\}.$$

The following theorem gives the theoretical foundation for the inductive step of the component-by-component construction.

Theorem 3.8 *Let n be a prime number. Suppose there exist $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1} \in [0,1]^d$ such that*

$$e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \leq \frac{1}{n} \prod_{j=1}^{d} (\beta_j + 4\gamma_j \zeta(\alpha)).$$

Then there exists $z_{d+1} \in \mathbb{Z}_n$ such that

$$e_{n,d+1}^2 (\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \leq \frac{1}{n} \prod_{j=1}^{d+1} (\beta_j + 4\gamma_j \zeta(\alpha)).$$

Such a z_{d+1} can be found by minimizing $e_{n,d+1}^2 (\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$ over the set $\mathbb{Z}_n$.

Proof. Suppose that $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ satisfy the assumed bound. For any $z_{d+1} \in \mathbb{Z}_n$, we have from Lemma 2.7 that

$$\begin{aligned}
& e_{n,d+1}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\
&= -\prod_{j=1}^{d+1} \beta_j + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i h (x_{i,j} - x_{k,j})}}{|h|^\alpha} \right) \right. \\
& \qquad \left. \times \left(\beta_{d+1} + \gamma_{d+1} {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i h (i-k) z_{d+1}/n}}{|h|^\alpha} \right) \right] \\
&= \beta_{d+1} e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
& \quad + \frac{\gamma_{d+1}}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i h (x_{i,j} - x_{k,j})}}{|h|^\alpha} \right) {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i h (i-k) z_{d+1}/n}}{|h|^\alpha} \right].
\end{aligned}$$

Next we average over the possible values of z_{d+1}, forming

$$
\begin{aligned}
&m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})\\
&:= \frac{1}{n-1}\sum_{z_{d+1}\in\mathbb{Z}_n} e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\\
&= \beta_{d+1}e^2_{n,d}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})\\
&\quad +\frac{\gamma_{d+1}}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_{i,j}-x_{k,j})}}{|h|^\alpha}\right)T_\alpha(i-k,n)\right],
\end{aligned}
$$

where $T_\alpha(k,n)$ is as given in Lemma 3.2 (with $z=z_{d+1}$). The second term in the expression for $m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})$ above can be bounded as follows:

$$
\begin{aligned}
&\frac{\gamma_{d+1}}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(x_{i,j}-x_{k,j})}}{|h|^\alpha}\right)T_\alpha(i-k,n)\right]\\
\le\;& \frac{\gamma_{d+1}}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{1}{|h|^\alpha}\right)|T_\alpha(i-k,n)|\right]\\
=\;& \frac{\gamma_{d+1}}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|T_\alpha(i-k,n)|\prod_{j=1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right).
\end{aligned}
$$

It follows from Lemma 3.2 that

$$
\begin{aligned}
\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|T_\alpha(i-k,n)| &= \sum_{i=0}^{n-1}|T_\alpha(0,n)|+\sum_{i=0}^{n-1}\sum_{\substack{k=0\\k\ne i}}^{n-1}|T_\alpha(i-k,n)|\\
&= n|2\zeta(\alpha)|+n(n-1)\left|-\frac{2\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right|\\
&= 2\zeta(\alpha)(2-n^{1-\alpha})n\\
&\le 4\zeta(\alpha)n.
\end{aligned}
$$

Hence

$$
\begin{aligned}
&m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})\\
&\le \beta_{d+1}e^2_{n,d}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})+\frac{4\gamma_{d+1}\zeta(\alpha)}{n}\prod_{j=1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right)\\
&\le \beta_{d+1}\times\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+4\gamma_j\zeta(\alpha)\right)+4\gamma_{d+1}\zeta(\alpha)\times\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+4\gamma_j\zeta(\alpha)\right)\\
&= \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j+4\gamma_j\zeta(\alpha)\right).
\end{aligned}
$$

Now since $m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})$ is the average of $e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ over all z_{d+1}, if we choose $z_{d+1}\in\mathbb{Z}_n$ to minimize $e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$, then this choice of z_{d+1} will satisfy

$$e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\le m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})\le\frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j+4\gamma_j\zeta(\alpha)\right).$$

This completes the proof. □

Corollary 3.9 *Let n be a prime number. We can construct $\boldsymbol{z}\in\mathbb{Z}_n^d$ component-by-component such that for all $s=1,\ldots,d$,*

$$e^2_{n,s}(z_1,\ldots,z_s)\le\frac{1}{n}\prod_{j=1}^{s}\left(\beta_j+4\gamma_j\zeta(\alpha)\right).$$

We can set $z_1=1$, and for s satisfying $2\le s\le d$, each z_s can be found by minimizing $e^2_{n,s}(z_1,\ldots,z_s)$ over the set $\mathbb{Z}_n$.

Proof. In one dimension, the only n-point lattice rule is the n-point rectangle rule having zero as a point. Thus we may take $z_1=1$. We have from Lemma 3.1 that

$$\begin{aligned}
e^2_{n,1}(1) &= -\beta_1+\frac{1}{n}\sum_{k=0}^{n-1}\left(\beta_1+\gamma_1\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i hk/n}}{|h|^\alpha}\right)\\
&= \frac{\gamma_1}{n}\sum_{k=0}^{n-1}\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i hk/n}}{|h|^\alpha}\\
&= \frac{\gamma_1}{n}\left[2\zeta(\alpha)+(n-1)\times T_\alpha(1,n)\right]\\
&= \frac{\gamma_1}{n}\left[2\zeta(\alpha)+(n-1)\times\left(-\frac{2\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right)\right]\\
&= \frac{2\gamma_1\zeta(\alpha)}{n^\alpha},
\end{aligned}\tag{3.2}$$

where $T_\alpha(1,n)$ is as given in Lemma 3.2. Note that (3.2) holds regardless of whether n is a prime number or not. Thus for all z_1 we have

$$e^2_{n,1}(z_1)=e^2_{n,1}(1)=\frac{2\gamma_1\zeta(\alpha)}{n^\alpha}\le\frac{1}{n}\left(\beta_1+4\gamma_1\zeta(\alpha)\right).$$

For each $s=2,\ldots,d$, it follows from Theorem 3.8 inductively with $d=s-1$ that z_s can be found by minimizing $e^2_{n,s}(z_1,\ldots,z_s)$ over the set $\mathbb{Z}_n$ and that this choice satisfies the desired bound. □

Corollary 3.9 leads us to the following algorithm for constructing a rank-1 lattice rule that achieves strong tractability error bounds in weighted Korobov spaces, that is, the square worst-case error satisfies the bound given in Theorem 2.9 with $a = 4\zeta(\alpha)$ and $b = 1$.

Algorithm 3.10 *Given n a prime number:*

1. *Set z_1, the first component of $\boldsymbol{z}$, to* 1.

2. *For $s = 2, 3, \ldots, d-1, d$, find $z_s \in \mathbb{Z}_n = \{1, 2, \ldots, n-1\}$ such that*

$$e_{n,s}^2(z_1, \ldots, z_s) = -\prod_{j=1}^{s} \beta_j + \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{s} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i k h z_j / n}}{|h|^\alpha} \right)$$

is minimized.

We see from the algorithm that when α is taken to be an even integer (so that the infinite sum is expressed as a Bernoulli polynomial), the cost of constructing a n-point rank-1 lattice rule for all dimensions up to d is approximately $O(n^2 d^2)$ operations. This can be reduced to $O(n^2 d)$ operations if we store the n products during the search, which would require $O(n)$ storage.

Chapter 4

Constructing Shifted Rank-1 Lattice Rules in Weighted Sobolev Spaces

We have shown in Chapter 3 that when the sum of γ_j/β_j is finite, the family of rank-1 lattice rules with a prime number of points is strongly tractable in weighted Korobov spaces, and the generating vector for a rule achieving the strong tractability bounds can be constructed by a component-by-component algorithm. Here we obtain similar results for weighted Sobolev spaces. We show that when n is prime, there exists a shifted rank-1 lattice rule with square worst-case error bounded by an expression of the desired form as given in Theorem 2.15. We then derive a similar component-by-component algorithm to construct the generating vector and the shift of such a rule.

4.1 The existence of good rules

We recall from Chapter 2 that weighted Sobolev spaces are tensor product reproducing kernel Hilbert spaces of non-periodic functions. The spaces are parameterized by a real vector $\boldsymbol{a} \in [0,1]^d$ (common choices are $\boldsymbol{a} = \mathbf{1}$ or

$\boldsymbol{a} = \frac{1}{2}$), and two sequences of positive weights $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ satisfying

$$\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots .$$

Throughout this chapter, we will consider the case of $\boldsymbol{a} = \mathbf{1}$. Shifted rank-1 lattice rules (see (1.7)) are QMC rules with quadrature points given by the set

$$\left\{ \left\{ \frac{i\boldsymbol{z}}{n} + \boldsymbol{\Delta} \right\} : i = 0, \ldots, n-1 \right\},$$

where $\boldsymbol{z} \in \mathcal{Z}_n^d$ is the 'generating vector' with $\mathcal{Z}_n$ given by (1.5) and $\boldsymbol{\Delta} \in [0,1)^d$ is the 'shift'.

In this section, we first give an explicit expression for the square worst-case error. Using the close relationship between weighted Sobolev spaces and weighted Korobov spaces, we give the expression for the mean square worst-case error when n is prime and derive an upper bound on the mean. With this upper bound, we prove the the existence of shifted rank-1 lattice rules that achieve strong tractability error bounds (see Theorem 2.15) in weighted Sobolev spaces.

4.1.1 Square worst-case error

Let $e_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta})$ denote the worst-case error of a shifted rank-1 lattice rule with generating vector $\boldsymbol{z}$ and shift $\boldsymbol{\Delta}$. We give the expression for $e_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta})$ in the lemma below.

Lemma 4.1 *We have*

$$\begin{aligned} & e_{n,d}^2(\boldsymbol{z}, \boldsymbol{\Delta}) \\ = & \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{3} \right) - \frac{2}{n} \sum_{i=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{2} \left(1 - \left\{ \frac{iz_j}{n} + \Delta_j \right\}^2 \right) \right) \\ & + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[1 - \max \left(\left\{ \frac{iz_j}{n} + \Delta_j \right\}, \left\{ \frac{kz_j}{n} + \Delta_j \right\} \right) \right] \right), \end{aligned}$$

Proof. The result follows directly from Lemma 2.16 with $\boldsymbol{x}_i = \left\{ \frac{i\boldsymbol{z}}{n} \right\}$. □

4.1.2 Mean and upper bound when n is prime

We define the mean square worst-case error over all values of $\boldsymbol{z} \in \mathcal{Z}_n^d$ and $\boldsymbol{\Delta} \in [0,1)^d$ by

$$M_{n,d} := \frac{1}{[\phi(n)]^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} \left(\int_{[0,1]^d} e_{n,d}^2(\boldsymbol{z}, \boldsymbol{\Delta}) \, \mathrm{d}\boldsymbol{\Delta} \right).$$

For simplicity, we choose n to be a prime number. The expressions for $M_{n,d}$ and its upper bound when n is prime are given in the next lemma.

Theorem 4.2 *Let n be a prime number. Then*

$$M_{n,d} = -\prod_{j=1}^d \left(\beta_j + \frac{\gamma_j}{3}\right) + \frac{1}{n} \prod_{j=1}^d \left(\beta_j + \frac{\gamma_j}{2}\right) + \frac{n-1}{n} \prod_{j=1}^d \left(\beta_j + \gamma_j \left(\frac{1}{3} + \frac{1}{6n}\right)\right).$$

Moreover,

$$M_{n,d} \le \min \left(\frac{2}{n} \prod_{j=1}^d \left(\beta_j + \frac{\gamma_j}{2}\right), \frac{1}{n} \prod_{j=1}^d \left(\beta_j + \frac{2\gamma_j}{3}\right) \right).$$

Proof. Let $e_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}}(\boldsymbol{z})$ denote the worst-case error for a rank-1 lattice rule with generating vector $\boldsymbol{z}$ in weighted Korobov spaces with $\alpha = 2$,

$$\hat{\beta}_j = \beta_j + \frac{\gamma_j}{3} \qquad \text{and} \qquad \hat{\gamma}_j = \frac{\gamma_j}{2\pi^2}.$$

Then it follows from Lemma 2.12 with $\boldsymbol{a} = \boldsymbol{1}$ and Lemma 2.4 with $\boldsymbol{x}_i = \left\{\frac{i\boldsymbol{z}}{n}\right\}$ that

$$\int_{[0,1]^d} e_{n,d}^2(\boldsymbol{z}, \boldsymbol{\Delta}) \, \mathrm{d}\boldsymbol{\Delta} = e_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}}^2(\boldsymbol{z}).$$

Thus

$$M_{n,d} = \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathbb{Z}_n^d} e_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}}^2(\boldsymbol{z}) = M_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}},$$

where we have from Theorem 3.3 and Theorem 3.6 that

$$\begin{aligned} M_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}} &= -\prod_{j=1}^d \hat{\beta}_j + \frac{1}{n} \prod_{j=1}^d \left(\hat{\beta}_j + 2\hat{\gamma}_j \zeta(2)\right) \\ &\quad + \frac{n-1}{n} \prod_{j=1}^d \left(\hat{\beta}_j - \frac{2\hat{\gamma}_j \zeta(2)(1-n^{-1})}{n-1}\right), \end{aligned}$$

and

$$M_{n,d,\hat{\boldsymbol{\beta}},\hat{\boldsymbol{\gamma}}} \le \min \left(\frac{2}{n} \prod_{j=1}^d \left(\hat{\beta}_j + 2\hat{\gamma}_j \zeta(2)\right), \frac{1}{n} \prod_{j=1}^d \left(\hat{\beta}_j + 4\hat{\gamma}_j \zeta(2)\right) \right).$$

Now since

$$\begin{aligned}
\hat{\beta}_j + 2\hat{\gamma}_j\zeta(2) &= \beta_j + \frac{\gamma_j}{3} + 2\frac{\gamma_j}{2\pi^2}\frac{\pi^2}{6} = \beta_j + \frac{\gamma_j}{2}, \\
\hat{\beta}_j + 4\hat{\gamma}_j\zeta(2) &= \beta_j + \frac{\gamma_j}{3} + 4\frac{\gamma_j}{2\pi^2}\frac{\pi^2}{6} = \beta_j + \frac{2\gamma_j}{3}, \\
\hat{\beta}_j - \frac{2\hat{\gamma}_j\zeta(2)(1-n^{-1})}{n-1} &= \beta_j + \frac{\gamma_j}{3} - \frac{2\frac{\gamma_j}{2\pi^2}\frac{\pi^2}{6}(1-n^{-1})}{n-1} = \beta_j + \gamma_j\left(\frac{1}{3} + \frac{1}{6n}\right),
\end{aligned}$$

the result follows. □

Corollary 4.3 *Let n be a prime number. Then there exist a choice of $\boldsymbol{z} \in \mathbb{Z}_n^d$ and a choice of $\boldsymbol{\Delta} \in [0,1)^d$ such that*

$$e_{n,d}^2(\boldsymbol{z}, \boldsymbol{\Delta}) \le \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j}{3}\right) \le \frac{1}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j).$$

Clearly the last bound in Corollary 4.3 is of the form given in Theorem 2.9 with $a = b = 1$. We thus conclude that *the family of shifted rank-1 lattice rules with a prime number of points is strongly tractable in weighted Sobolev spaces if and only if*

$$\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty.$$

4.2 Component-by-component construction

In this section we prove that the generating vector and the shift of a shifted rank-1 lattice rule achieving the strong tractability error bounds can be constructed component-by-component.

Let $e_{n,d}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1})$ denote the worst-case error for a QMC rule with the set of points $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}\}$, and let $e_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$ denote the worst-case error for a QMC rule with the set of points

$$\left\{\left(\boldsymbol{x}_i, \left\{\frac{iz_{d+1}}{n} + \Delta_{d+1}\right\}\right) : 0 \le i \le n-1\right\}.$$

We define the mean of $e_{n,d+1}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$ taken over all values of $\Delta_{d+1} \in [0,1)$:

$$\omega_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) := \int_0^1 e_{n,d+1}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})\,\mathrm{d}\Delta_{d+1}.$$

We define also a discrete form of the mean $\omega_{n,d+1}$:

$$\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}) := \frac{1}{n}\sum_{m=1}^{n} e_{n,d+1}^2\left(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\tfrac{2m-1}{2n}\right).$$

Lemma 4.4 below gives the expression for the mean $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$, while Lemma 4.5 shows that the discrete mean $\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ is less than $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$. Note that both these results hold regardless of whether n is a prime number or not.

In these two lemmas, the notation $\boldsymbol{x}\in[0,1]^0$ will be taken to mean that $\boldsymbol{x}$ does not exist.

Lemma 4.4 *For $d\geq 0$, given $\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}\in[0,1]^d$ and $z_{d+1}\in\mathcal{Z}_n$, we have*

$$\begin{aligned}
&\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\\
&= \prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{3}\right) - \frac{2}{n}\sum_{i=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\left(1-x_{i,j}^2\right)\right)\left(\beta_{d+1}+\frac{\gamma_{d+1}}{3}\right)\right]\\
&\quad+\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[1-\max\left(x_{i,j},x_{k,j}\right)\right]\right)\right.\\
&\qquad\qquad\left.\times\left(\beta_{d+1}+\gamma_{d+1}\left[\frac{1}{3}+B_2\left(\left\{\frac{(i-k)z_{d+1}}{n}\right\}\right)\right]\right)\right].
\end{aligned}$$

Proof. For any $\Delta_{d+1}\in[0,1)$, we have from Lemma 2.16 that

$$\begin{aligned}
&e_{n,d+1}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})\\
&= \prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{3}\right) - \frac{2}{n}\sum_{i=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\left(1-x_{i,j}^2\right)\right)\right.\\
&\qquad\qquad\left.\times\left(\beta_{d+1}+\frac{\gamma_{d+1}}{2}\left(1-\left\{\frac{iz_{d+1}}{n}+\Delta_{d+1}\right\}^2\right)\right)\right]\\
&\quad+\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[1-\max\left(x_{i,j},x_{k,j}\right)\right]\right)\right.\\
&\quad\left.\times\left(\beta_{d+1}+\gamma_{d+1}\left[1-\max\left(\left\{\frac{iz_{d+1}}{n}+\Delta_{d+1}\right\},\left\{\frac{kz_{d+1}}{n}+\Delta_{d+1}\right\}\right)\right]\right)\right].
\end{aligned}$$

By definition,

$$\begin{aligned}
&\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\\
&= \prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{3}\right)-\frac{2}{n}\sum_{i=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\left(1-x_{i,j}^2\right)\right)\right.\\
&\qquad\qquad \left.\times\left(\beta_{d+1}+\frac{\gamma_{d+1}}{2}\left(1-\int_0^1\left\{\frac{iz_{d+1}}{n}+\Delta_{d+1}\right\}^2\mathrm{d}\Delta_{d+1}\right)\right)\right]\\
&\quad +\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[1-\max\left(x_{i,j},x_{k,j}\right)\right]\right)\left(\beta_{d+1}+\gamma_{d+1}\right.\right.\\
&\qquad\qquad \left.\left.\times\left[1-\int_0^1\max\left(\left\{\frac{iz_{d+1}}{n}+\Delta_{d+1}\right\},\left\{\frac{kz_{d+1}}{n}+\Delta_{d+1}\right\}\right)\mathrm{d}\Delta_{d+1}\right]\right)\right].
\end{aligned}$$

For any $x,y\in\mathbb{R}$, it may be verified that

$$\int_0^1\{x+\Delta\}^2\,\mathrm{d}\Delta=\frac{1}{3}\quad\text{and}\quad\int_0^1\max(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta=\frac{2}{3}-B_2(|x-y|).$$

Since

$$B_2\left(\left|\left\{\frac{iz_{d+1}}{n}\right\}-\left\{\frac{kz_{d+1}}{n}\right\}\right|\right)=B_2\left(\left\{\frac{(i-k)z_{d+1}}{n}\right\}\right),$$

the result follows. □

Lemma 4.5 *For $d\geq 0$, given $\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}\in[0,1]^d$ and $z_{d+1}\in\mathcal{Z}_n$, we have*

$$\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\leq\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}).$$

Proof. For any $x,y\in\mathbb{R}$, we have

$$\int_0^1\max\left(\{x+\Delta\},\{y+\Delta\}\right)\mathrm{d}\Delta=\sum_{m=1}^{n}\int_{\frac{m-1}{n}}^{\frac{m}{n}}\max\left(\{x+\Delta\},\{y+\Delta\}\right)\mathrm{d}\Delta$$

and

$$\int_0^1\{x+\Delta\}^2\,\mathrm{d}\Delta=\sum_{m=1}^{n}\int_{\frac{m-1}{n}}^{\frac{m}{n}}\{x+\Delta\}^2\,\mathrm{d}\Delta.$$

We see from Lemma 4.4 that these two integrals appear in the expression of $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$, with x and y being multiples of $\frac{1}{n}$. As a result, the values $\max(\{x+\Delta\},\{y+\Delta\})$ and $\{x+\Delta\}^2$ are continuous and differentiable on each sub-interval $[\frac{m-1}{n},\frac{m}{n}]$ of length $\frac{1}{n}$. Moreover, $\max(\{x+\Delta\},\{y+\Delta\})$

is linear on each sub-interval and so the result of applying the midpoint rule on each sub-interval is exact. Thus

$$\int_0^1 \max\left(\{x+\Delta\},\{y+\Delta\}\right)\,\mathrm{d}\Delta = \frac{1}{n}\sum_{m=1}^{n}\max\left(\left\{x+\tfrac{2m-1}{2n}\right\},\left\{y+\tfrac{2m-1}{2n}\right\}\right).$$

On the other hand, $\{x+\Delta\}^2$ is quadratic with a positive second derivative on each sub-interval and so upon applying the mid-point rule, we have for $m = 1, \ldots, n$,

$$\int_{\frac{m-1}{n}}^{\frac{m}{n}} \{x+\Delta\}^2\,\mathrm{d}\Delta > \frac{1}{n}\left\{x+\tfrac{2m-1}{2n}\right\}^2.$$

Hence

$$\int_0^1 \{x+\Delta\}^2\,\mathrm{d}\Delta > \frac{1}{n}\sum_{m=1}^{n}\left\{x+\tfrac{2m-1}{2n}\right\}^2.$$

Now since the discrete form $\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ is just the approximation to $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ obtained by the composite mid-point rule with spacing $\frac{1}{n}$, the result follows. □

In Theorem 4.6 below, we give the theoretical foundation for the inductive step of the component-by-component construction. The proof of Theorem 4.6 makes use of the previous two lemmas.

Theorem 4.6 *Let n be a prime number. Suppose there exist $\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1} \in [0,1]^d$ such that*

$$e_{n,d}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \le \frac{1}{n}\prod_{j=1}^{d}(\beta_j+\gamma_j).$$

Then there exist $z_{d+1} \in \mathbb{Z}_n$ and $\Delta_{d+1} \in [0,1)$ such that

$$e_{n,d+1}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1}) \le \frac{1}{n}\prod_{j=1}^{d+1}(\beta_j+\gamma_j).$$

A pair (z_{d+1},Δ_{d+1}) that achieves this bound can be found by first finding a $z_{d+1} \in \left\{1,2,\ldots,\frac{n-1}{2}\right\}$ that minimizes $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ and then (with this z_{d+1} fixed) finding a $\Delta_{d+1} \in \left\{\frac{2m-1}{2n} : m = 1,\ldots,n\right\}$ that minimizes $e_{n,d+1}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})$.

Proof. Suppose that $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ satisfy the assumed bound. For any $z_{d+1} \in \mathbb{Z}_n$, it follows from Lemma 4.4 and Lemma 2.16 that

$$\begin{aligned}
&\omega_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&+ \frac{\gamma_{d+1}}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} (\beta_j + \gamma_j [1 - \max(x_{i,j}, x_{k,j})]) \, B_2 \left(\left\{ \frac{(i-k) z_{d+1}}{n} \right\} \right) \right],
\end{aligned}$$

where we can write

$$B_2 \left(\left\{ \frac{(i-k) z_{d+1}}{n} \right\} \right) = \frac{1}{2\pi^2} \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h (i-k) z_{d+1}/n}}{h^2},$$

using (2.8) with $\alpha = 2$. Now we average this over all possible values of $z_{d+1} \in \mathbb{Z}_n$, forming

$$\begin{aligned}
&m_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&:= \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} \omega_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&\quad + \frac{\gamma_{d+1}}{2\pi^2 n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} (\beta_j + \gamma_j [1 - \max(x_{i,j}, x_{k,j})]) \, T_2(i-k, n) \right] \\
&\leq \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&\quad + \frac{\gamma_{d+1}}{2\pi^2 n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} |T_2(i-k, n)| \prod_{j=1}^{d} (\beta_j + \gamma_j),
\end{aligned}$$

where $T_2(k, n)$ is as given in Lemma 3.2 with $\alpha = 2$ and it follows from the proof of Theorem 3.8 with $\alpha = 2$ that

$$\sum_{i=0}^{n-1} \sum_{k=0}^{n-1} |T_2(i-k, n)| \leq 4\zeta(2) n = \frac{2\pi^2 n}{3}.$$

Hence

$$\begin{aligned}
&m_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&\leq \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) \times \frac{1}{n} \prod_{j=1}^{d} (\beta_j + \gamma_j) + \frac{\gamma_{d+1}}{3n} \prod_{j=1}^{d} (\beta_j + \gamma_j) \\
&\leq \frac{1}{n} \prod_{j=1}^{d+1} (\beta_j + \gamma_j).
\end{aligned}$$

Since $m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})$ is the average of $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ over all z_{d+1}, if we choose $z_{d+1}\in\mathbb{Z}_n$ to minimize $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$, then this choice of z_{d+1} will satisfy

$$\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})\le m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})\le\frac{1}{n}\prod_{j=1}^{d+1}(\beta_j+\gamma_j)\,.$$

Now for this z_{d+1}, the expression $\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ is the average of $e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})$ over all Δ_{d+1} in the set $\left\{\frac{2m-1}{2n}:m=1,\ldots,n\right\}$. Therefore if we choose Δ_{d+1} from this finite set to minimize the expression $e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})$, then this choice of Δ_{d+1} will satisfy

$$e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})\le\widetilde{\omega}_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}),$$

and in turn it follows from Lemma 4.5 that

$$e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1},\Delta_{d+1})\le\frac{1}{n}\prod_{j=1}^{d+1}(\beta_j+\gamma_j).$$

The second degree Bernoulli polynomial has the property that

$$B_2(\{x\})=B_2(1-\{x\}),$$

which leads to

$$\omega_{n,d+1}(\boldsymbol{z},\boldsymbol{\Delta};z_{d+1})=\omega_{n,d+1}(\boldsymbol{z},\boldsymbol{\Delta};n-z_{d+1}).$$

Thus the search of z_{d+1} can be restricted to the set $\left\{1,2,\ldots,\frac{n-1}{2}\right\}$. This completes the proof. □

Corollary 4.7 *Let n be a prime number. We can construct $\boldsymbol{z}\in\mathbb{Z}_n^d$ and $\boldsymbol{\Delta}\in[0,1)^d$ component-by-component such that for all $s=1,\ldots,d$,*

$$e^2_{n,s}\left((z_1,\ldots,z_s),(\Delta_1,\ldots,\Delta_s)\right)\le\frac{1}{n}\prod_{j=1}^{s}(\beta_j+\gamma_j).$$

We can set $z_1=1$, and find Δ_1 in the set $\left\{\frac{2m-1}{2n}:m=1,\ldots,n\right\}$ to minimize $e^2_{n,1}(1,\Delta_1)$. For s satisfying $2\le s\le d$, each pair (z_s,Δ_s) can be found by first *finding a* z_s *in* $\left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ *that minimizes*

$$\begin{aligned} &\omega_{n,s}\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1}); z_s\right) \\ &= \left(\beta_s + \frac{\gamma_s}{3}\right) e^2_{n,s-1}\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1})\right) \\ &\quad + \frac{\gamma_s}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{s-1} \left(\beta_j + \gamma_j \left[1 - \max\left(\left\{\frac{iz_j}{n} + \Delta_j\right\}, \left\{\frac{kz_j}{n} + \Delta_j\right\}\right)\right]\right) \right. \\ &\qquad\qquad \left. \times B_2\left(\left\{\frac{(i-k)z_s}{n}\right\}\right)\right], \end{aligned}$$

and then (with this z_s *fixed) finding a* Δ_s *in* $\left\{\frac{2m-1}{2n} : m = 1, \ldots, n\right\}$ *that minimizes* $e^2_{n,s}\left((z_1, \ldots, z_s), (\Delta_1, \ldots, \Delta_s)\right)$.

Proof. As mentioned earlier, the n-point rectangle rule is the only n-point lattice rule in one dimension and hence we may take $z_1 = 1$. We have from Lemma 4.4 with $d = 0$ and $z_1 = 1$ that

$$\omega_{n,1}(1) = \frac{\gamma_1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} B_2\left(\left\{\frac{i-k}{n}\right\}\right) = \frac{\gamma_1}{n} \sum_{i=0}^{n-1} B_2\left(\frac{i}{n}\right).$$

By recalling that $B_2(x) = x^2 - x + \frac{1}{6}$ and using the well-known sums for the first $n-1$ positive integers and the squares of the first $n-1$ positive integers, we obtain

$$\frac{1}{n} \sum_{i=0}^{n-1} B_2\left(\frac{i}{n}\right) = \frac{1}{n} \sum_{i=0}^{n-1} \left[\left(\frac{i}{n}\right)^2 - \left(\frac{i}{n}\right) + \frac{1}{6}\right] = \frac{1}{6n^2}. \tag{4.1}$$

Thus

$$\omega_{n,1}(1) = \frac{\gamma_1}{6n^2}, \tag{4.2}$$

which holds regardless of whether or not n is a prime number. Now since $\widetilde{\omega}_{n,1}(1)$ is the average of $e^2_{n,1}(1, \Delta_1)$ over all Δ_1 in the set $\left\{\frac{2m-1}{2n} : m = 1, \ldots, n\right\}$ and $\widetilde{\omega}_{n,1}(1) \le \omega_{n,1}(1)$, if we choose Δ_1 from this finite set to minimize $e^2_{n,1}(1, \Delta_1)$ then this choice of Δ_1 will satisfy

$$e^2_{n,1}(1, \Delta_1) \le \widetilde{\omega}_{n,1}(1) \le \omega_{n,1}(1) = \frac{\gamma_1}{6n^2} \le \frac{1}{n}\left(\beta_1 + \gamma_1\right).$$

For each $s = 2, \ldots, d$, the result follows from Theorem 4.6 inductively with $d = s - 1$. □

Corollary 4.7 leads us to the following algorithm for constructing shifted rank-1 lattice rules that achieve strong tractability error bounds in weighted Sobolev spaces.

Algorithm 4.8 *Given n a prime number:*

1. *Set z_1, the first component of $\boldsymbol{z}$, to* 1.

2. *Find $\Delta_1 \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize*

$$\begin{aligned} e_{n,1}^2(1,\Delta_1) &= \frac{\gamma_1}{3} + \frac{\gamma_1}{n}\left\{\tfrac{i}{n} + \Delta_1\right\}^2 \\ &\quad -\frac{\gamma_1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\max\left(\left\{\tfrac{i}{n}+\Delta_1\right\},\left\{\tfrac{k}{n}+\Delta_1\right\}\right). \end{aligned}$$

3. *For $s = 2, 3, \ldots, d-1, d$, do the following:*

   (a) *Find $z_s \in \{1, 2, \ldots, \frac{n-1}{2}\}$ to minimize*

$$\begin{aligned} &\omega_{n,s}\left((z_1,\ldots,z_{s-1}),(\Delta_1,\ldots,\Delta_{s-1});z_s\right) \\ &= \left(\beta_s + \frac{\gamma_s}{3}\right)e_{n,s-1}^2\left((z_1,\ldots,z_{s-1}),(\Delta_1,\ldots,\Delta_{s-1})\right) \\ &\quad + \frac{\gamma_s}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[1 - \max\left(\left\{\tfrac{iz_j}{n}+\Delta_j\right\},\left\{\tfrac{kz_j}{n}+\Delta_j\right\}\right)\right]\right)\right. \\ &\qquad\qquad \left. \times B_2\left(\left\{\tfrac{(i-k)z_s}{n}\right\}\right)\right]. \end{aligned}$$

   (b) *Find $\Delta_s \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize*

$$\begin{aligned} &e_{n,s}^2\left((z_1,\ldots,z_s),(\Delta_1,\ldots,\Delta_s)\right) \\ &= \prod_{j=1}^{s}\left(\beta_j + \frac{\gamma_j}{3}\right) - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left[\beta_j + \frac{\gamma_j}{2}\left(1 - \left\{\tfrac{iz_j}{n}+\Delta_j\right\}^2\right)\right] \\ &\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[\beta_j + \gamma_j\left(1 - \max\left(\left\{\tfrac{iz_j}{n}+\Delta_j\right\},\left\{\tfrac{kz_j}{n}+\Delta_j\right\}\right)\right)\right]. \end{aligned}$$

We see from the algorithm that the cost of constructing a rule for all dimensions up to d is approximately $O(n^3d^2)$ operations. This can be reduced to $O(n^3d)$ operations at the expense of $O(n^2)$ storage.

Chapter 5

Constructing Lattice Rules with a Composite Number of Points

Both the constructions given in Chapter 3 and Chapter 4 made the assumption that the number of points n was a prime number. Here we extend the theories and the algorithms from Chapter 3 and Chapter 4 to lattice rules with a composite number of points. The analyses in this chapter are much more complicated. The proofs use techniques similar to those of [6] in which Disney studied the error bounds for rank-1 lattice rules with a composite number of points in unweighted Korobov spaces.

5.1 Rank-1 lattice rules in weighted Korobov spaces

In this section, we generalize the results from Chapter 3 to rank-1 lattice rules with a composite number of points for integrands in weighted Korobov spaces.

5.1.1 Mean for general n

We derive the expression for the mean square worst-case error when n is a composite number. Definition 5.1 and Lemma 5.2 are essential for our derivation. They are both taken from [6].

Definition 5.1 *For $\alpha > 1$ and $1 \le k \le n$, we define $S_\alpha(k,n)$ by*

$$S_\alpha(k,n) := \frac{1}{\phi(n)n^{\alpha-1}} \sum_{a|n} \mu(a)a^{\alpha-1}\Big[\gcd(n/a,k)\Big]^\alpha,$$

where ϕ is Euler's function and μ is the Mobius function defined by

$$\mu(a) := \begin{cases} 1, & \text{if } a = 1, \\ (-1)^i, & \text{if } a \text{ is a product of } i \text{ distinct primes}, \\ 0, & \text{otherwise.} \end{cases}$$

Lemma 5.2 *For $\alpha > 1$ and $1 \le k \le n$,*

$$\frac{1}{\phi(n)} \sum_{\substack{z=1 \\ \gcd(z,n)=1}}^{n-1} \sideset{}{'}\sum_{h=-\infty}^{\infty} \frac{e^{2\pi i h k z/n}}{|h|^\alpha} = 2\zeta(\alpha)S_\alpha(k,n),$$

where $S_\alpha(k,n)$ is as given in Definition 5.1.

Proof. Let

$$\Upsilon := \frac{1}{\phi(n)} \sum_{\substack{z=1 \\ \gcd(z,n)=1}}^{n-1} \sideset{}{'}\sum_{h=-\infty}^{\infty} \frac{e^{2\pi i h k z/n}}{|h|^\alpha} = \frac{1}{\phi(n)} \sideset{}{'}\sum_{h=-\infty}^{\infty} \left(\frac{1}{|h|^\alpha} \sum_{\substack{z=1 \\ \gcd(z,n)=1}}^{n-1} e^{2\pi i h k z/n} \right).$$

The Mobius function μ in Definition 5.1 has the property (see Theorem 6-5 of [1]) that

$$\sum_{a|m} \mu(a) = \begin{cases} 1, & \text{if } m = 1, \\ 0, & \text{otherwise.} \end{cases}$$

Thus we can write

$$\begin{aligned} \sum_{\substack{z=1 \\ \gcd(z,n)=1}}^{n-1} e^{2\pi i h k z/n} = \sum_{\substack{z=1 \\ \gcd(z,n)=1}}^{n} e^{2\pi i h k z/n} &= \sum_{z=1}^{n} \left(e^{2\pi i h k z/n} \sum_{a|\gcd(z,n)} \mu(a) \right) \\ &= \sum_{z=1}^{n} \sum_{a|\gcd(z,n)} e^{2\pi i h k z/n}\mu(a), \end{aligned}$$

which can be rearranged as follows:

$$\begin{aligned} \sum_{z=1}^{n} \sum_{a|\gcd(z,n)} e^{2\pi i h k z/n}\mu(a) &= \sum_{z=1}^{n} \sum_{\substack{a|n \\ a|z}} e^{2\pi i h k z/n}\mu(a) \\ &= \sum_{a|n} \sum_{\substack{z=1 \\ z\equiv 0 \ (\bmod\ a)}}^{n} e^{2\pi i h k z/n}\mu(a) \\ &= \sum_{a|n} \sum_{m=1}^{n/a} e^{2\pi i h k m a/n}\mu(a). \end{aligned}$$

From this we have

$$\begin{aligned}\Upsilon &= \frac{1}{\phi(n)}\sum_{h=-\infty}^{\infty}{}' \left(\frac{1}{|h|^\alpha}\sum_{a|n}\sum_{m=1}^{n/a} e^{2\pi i hkma/n}\mu(a)\right)\\ &= \frac{1}{\phi(n)}\sum_{a|n}\left[\mu(a)\sum_{h=-\infty}^{\infty}{}'\left(\frac{1}{|h|^\alpha}\sum_{m=1}^{n/a} e^{2\pi i hkma/n}\right)\right].\end{aligned}$$

Now

$$\sum_{m=1}^{n/a} e^{2\pi i hkma/n} = \sum_{m=1}^{n/a}\left(e^{2\pi i hk/(n/a)}\right)^m = \begin{cases}\frac{n}{a}, & \text{if } hk\equiv 0 \pmod{n/a},\\ 0, & \text{otherwise.}\end{cases}$$

Since $hk\equiv 0 \pmod{n/a}$ if and only if $h\equiv 0 \,(\bmod\, \frac{n}{a\gcd(n/a,k)})$, this leads to

$$\begin{aligned}\Upsilon &= \frac{1}{\phi(n)}\sum_{a|n}\left(\frac{\mu(a)\,n}{a}\sum_{\substack{h=-\infty\\ h\equiv 0\,(\bmod\, \frac{n}{a\gcd(n/a,k)})}}^{\infty}{}' \frac{1}{|h|^\alpha}\right)\\ &= \frac{1}{\phi(n)}\sum_{a|n}\left(\frac{\mu(a)\,n}{a}\sum_{m=-\infty}^{\infty}{}'\frac{1}{\left|\frac{mn}{a\gcd(n/a,k)}\right|^\alpha}\right)\\ &= \frac{1}{\phi(n)}\sum_{a|n}\left[\frac{\mu(a)\,n}{a}\left(\frac{a\gcd(n/a,k)}{n}\right)^\alpha\sum_{m=-\infty}^{\infty}{}'\frac{1}{|m|^\alpha}\right]\\ &= 2\zeta(\alpha)\times\frac{1}{\phi(n)n^{\alpha-1}}\sum_{a|n}\mu(a)a^{\alpha-1}\Big[\gcd(n/a,k)\Big]^\alpha = 2\zeta(\alpha)S_\alpha(k,n).\end{aligned}$$

This completes the proof. □

Now we give the expression of $M_{n,d}$ for a general n.

Theorem 5.3 [cf. Theorem 3.3] *We have*

$$M_{n,d} = -\prod_{j=1}^d \beta_j + \frac{1}{n}\sum_{k=1}^n\prod_{j=1}^d\left(\beta_j + 2\gamma_j\zeta(\alpha)S_\alpha(k,n)\right),$$

where $S_\alpha(k,n)$ is as given in Definition 5.1.

Proof. By the definition of the mean and Lemma 3.1, we have

$$\begin{aligned}M_{n,d} &= \frac{1}{[\phi(n)]^d}\sum_{z\in\mathcal{Z}_n^d}\left[-\prod_{j=1}^d\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^d\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i hkz_j/n}}{|h|^\alpha}\right)\right]\\ &= \frac{1}{[\phi(n)]^d}\sum_{z\in\mathcal{Z}_n^d}\left[-\prod_{j=1}^d\beta_j + \frac{1}{n}\sum_{k=1}^{n}\prod_{j=1}^d\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i hkz_j/n}}{|h|^\alpha}\right)\right]\\ &= -\prod_{j=1}^d\beta_j + \frac{1}{n}\sum_{k=1}^{n}\prod_{j=1}^d\left(\beta_j+\gamma_j\times\frac{1}{\phi(n)}\sum_{\substack{z=1\\ \gcd(z,n)=1}}^{n-1}\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i hkz/n}}{|h|^\alpha}\right).\end{aligned}$$

The result now follows from Lemma 5.2. □

5.1.2 Upper bound for general n

To obtain an upper bound on the mean square worst-case error, we need to make use of the following lemma. The proof for this lemma uses arguments from [6].

Lemma 5.4 *Let $S_\alpha(k,n)$ be as given in Definition 5.1. Then for $\lambda \in \mathbb{Z}^+$,*

$$\sum_{k=1}^{n} \left[S_\alpha(k,n)\right]^\lambda \le \frac{n}{\phi(n)} \le 2^c,$$

where c is the number of distinct prime factors of n.

Proof. Given $\alpha > 1$ and $\lambda \in \mathbb{Z}^+$, let

$$F_{\alpha,\lambda}(n) := \sum_{k=1}^{n} \left[S_\alpha(k,n)\right]^\lambda .$$

Now suppose $\gcd(m,n) = 1$, $a|m$, and $a'|n$. Then

$$\gcd(m/a, i)\gcd(n/a', j) = \gcd(mn/aa', ni + mj),$$

which, by the definition of S_α, leads to

$$\begin{aligned}
& S_\alpha(i,m)S_\alpha(j,n) \\
&= \frac{1}{\phi(m)\phi(n)(mn)^{\alpha-1}} \\
&\qquad \times \sum_{a|m}\sum_{a'|n} \left(\mu(a)\mu(a')(aa')^{\alpha-1}\Big[\gcd(m/a,i)\gcd(n/a',j)\Big]^\alpha\right) \\
&= \frac{1}{\phi(mn)(mn)^{\alpha-1}} \sum_{aa'|mn} \left(\mu(aa')(aa')^{\alpha-1}\Big[\gcd(mn/aa', ni+mj)\Big]^\alpha\right) \\
&= S_\alpha(ni+mj, mn).
\end{aligned}$$

Thus for m and n relatively prime, we have

$$\begin{aligned}
F_{\alpha,\lambda}(m)F_{\alpha,\lambda}(n) &= \sum_{i=1}^{m} \left[S_\alpha(i,m)\right]^\lambda \sum_{j=1}^{n} \left[S_\alpha(j,n)\right]^\lambda \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} \left[S_\alpha(i,m)S_\alpha(j,n)\right]^\lambda \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} \left[S_\alpha(ni+mj,mn)\right]^\lambda \\
&= \sum_{i=1}^{mn} \left[S_\alpha(i,mn)\right]^\lambda \\
&= F_{\alpha,\lambda}(mn).
\end{aligned}$$

This shows that F is a multiplicative arithmetic function, that is, if $n = p_1^{q_1} p_2^{q_2} \cdots p_c^{q_c}$, where $p_1, \ldots, p_c$ are distinct primes, then

$$F_{\alpha,\lambda}(n) = \prod_{t=1}^{c} F_{\alpha,\lambda}(p_t^{q_t}).$$

For p a prime number and $q \geq 1$, the value of Euler's function for p^q is given by

$$\phi(p^q) = p^q - p^{q-1} = p^{q-1}(p-1),$$

and the divisors of p^q are $1, p, p^2, \ldots, p^q$. By the definition of the Mobius function,

$$\mu(1) = 1, \mu(p) = -1, \text{ and } \mu(p^i) = 0 \text{ for } 2 \leq i \leq q.$$

It follows from Definition 5.1 that

$$\begin{aligned} S_\alpha(k, p^q) &= \frac{1}{p^{q-1}(p-1)(p^q)^{\alpha-1}} \sum_{a|p^q} \mu(a) a^{\alpha-1} \left[\gcd(p^q/a, k)\right]^\alpha \\ &= \frac{1}{p^{q-1}(p-1)(p^q)^{\alpha-1}} \left(\left[\gcd(p^q, k)\right]^\alpha - p^{\alpha-1} \left[\gcd(p^{q-1}, k)\right]^\alpha \right) \\ &= \frac{1}{p^{\alpha q-1}(p-1)} J(k), \end{aligned}$$

where

$$\begin{aligned} J(k) &:= \left[\gcd(p^q, k)\right]^\alpha - p^{\alpha-1} \left[\gcd(p^{q-1}, k)\right]^\alpha \\ &= \begin{cases} p^{\alpha q-1}(p-1), & \text{if } k = p^q, \\ 1 - p^{\alpha-1}, & \text{if } \gcd(p^q, k) = 1, \\ p^{\alpha i}(1 - p^{\alpha-1}), & \text{if } \gcd(p^q, k) = p^i,\ 1 \leq i \leq q-1. \end{cases} \end{aligned}$$

Thus

$$\begin{aligned} &F_{\alpha,\lambda}(p^q) \\ &= \sum_{k=1}^{p^q} \left[S_\alpha(k, p^q)\right]^\lambda \\ &= \frac{1}{p^{(\alpha q-1)\lambda}(p-1)^\lambda} \sum_{k=1}^{p^q} \left[J(k)\right]^\lambda \\ &= \frac{1}{p^{(\alpha q-1)\lambda}(p-1)^\lambda} \left(\left[J(p^q)\right]^\lambda + \sum_{\substack{k=1 \\ \gcd(p^q,k)=1}}^{p^q} \left[J(k)\right]^\lambda + \sum_{i=1}^{q-1} \sum_{\substack{k=1 \\ \gcd(p^q,k)=p^i}}^{p^q} \left[J(k)\right]^\lambda \right). \end{aligned}$$

Now $\left[J(p^q)\right]^\lambda = p^{(\alpha q-1)\lambda}(p-1)^\lambda$ and

$$\sum_{\substack{k=1\\ \gcd(p^q,k)=1}}^{p^q} \left[J(k)\right]^\lambda = \sum_{\substack{k=1\\ \gcd(p^q,k)=1}}^{p^q} \left(1-p^{\alpha-1}\right)^\lambda = \left(p^q-p^{q-1}\right)\left(1-p^{\alpha-1}\right)^\lambda$$

$$= p^{q-1}(p-1)\left(1-p^{\alpha-1}\right)^\lambda,$$

while

$$\begin{aligned}
\sum_{i=1}^{q-1} \sum_{\substack{k=1\\ \gcd(p^q,k)=p^i}}^{p^q} \left[J(k)\right]^\lambda &= \sum_{i=1}^{q-1} \sum_{\substack{k=1\\ \gcd(p^q,k)=p^i}}^{p^q} p^{(\alpha i)\lambda}(1-p^{\alpha-1})^\lambda \\
&= \sum_{i=1}^{q-1}(p^{q-i}-p^{q-i-1})p^{(\alpha i)\lambda}(1-p^{\alpha-1})^\lambda \\
&= p^{q-1}(p-1)(1-p^{\alpha-1})^\lambda \sum_{i=1}^{q-1} p^{\alpha i\lambda - i} \\
&= p^{q-1}(p-1)(1-p^{\alpha-1})^\lambda \sum_{i=1}^{q-1} (p^{\alpha\lambda-1})^i \\
&= p^{q-1}(p-1)(1-p^{\alpha-1})^\lambda \frac{p^{(\alpha\lambda-1)q}-p^{\alpha\lambda-1}}{p^{\alpha\lambda-1}-1}.
\end{aligned}$$

Upon combining these expressions together and doing some algebraic manipulations, we obtain

$$\begin{aligned}
F_{\alpha,\lambda}(p^q) &= \frac{1}{p^{(\alpha q-1)\lambda}(p-1)^\lambda}\Bigg[p^{(\alpha q-1)\lambda}(p-1)^\lambda + p^{q-1}(p-1)\left(1-p^{\alpha-1}\right)^\lambda \\
&\qquad + p^{q-1}(p-1)(1-p^{\alpha-1})^\lambda \frac{p^{(\alpha\lambda-1)q}-p^{\alpha\lambda-1}}{p^{\alpha\lambda-1}-1}\Bigg] \\
&= 1 + (-1)^\lambda \frac{\left(1-\frac{1}{p^{\alpha-1}}\right)^\lambda \left(1-\frac{1}{p^{(\alpha\lambda-1)q}}\right)}{(p-1)^{\lambda-1}\left(1-\frac{1}{p^{\alpha\lambda-1}}\right)} \\
&\le 1+\frac{1}{p-1} = \frac{p}{p-1}.
\end{aligned}$$

Hence

$$F_{\alpha,\lambda}(n) = \prod_{t=1}^{c} F_{\alpha,\lambda}(p_t^{q_t}) \le \prod_{t=1}^{c} \frac{p_t}{p_t-1} = \frac{n}{\phi(n)} \le \prod_{t=1}^{c} 2 = 2^c.$$

This completes the proof. □

In Theorem 5.5 below, we derive an upper bound for the mean $M_{n,d}$ given by Theorem 5.3.

Theorem 5.5 [cf. Theorem 3.6] *We have*

$$M_{n,d} \le \min\left(\frac{1}{\phi(n)}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right), \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right)\right),$$

where c is the number of distinct prime factors of n.

Proof. Using Lemma 3.5, we can write $M_{n,d}$ from Theorem 5.3 as

$$\begin{aligned} M_{n,d} &= -\prod_{j=1}^{d}\beta_j + \frac{1}{n}\sum_{k=1}^{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)S_\alpha(k,n)\right) \\ &= \frac{1}{n}\sum_{k=1}^{n}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)S_\alpha(k,n)\right)\right) \\ &= \frac{1}{n}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(\sum_{k=1}^{n}\left[S_\alpha(k,n)\right]^{|\mathfrak{u}|}\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right). \end{aligned}$$

Since $1 \le |\mathfrak{u}| \le d$, we have from Lemma 5.4 that

$$\sum_{k=1}^{n}\left[S_\alpha(k,n)\right]^{|\mathfrak{u}|} \le \frac{n}{\phi(n)} \le 2^c.$$

Thus we can obtain the first bound as follows:

$$\begin{aligned} M_{n,d} &\le \frac{1}{n}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(\frac{n}{\phi(n)}\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right) \\ &= \frac{1}{\phi(n)}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right) \\ &= \frac{1}{\phi(n)}\left(\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) - \prod_{j=1}^{d}\beta_j\right) \\ &\le \frac{1}{\phi(n)}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right). \end{aligned}$$

To obtain the second bound, we can proceed as follows:

$$\begin{aligned} M_{n,d} &\le \frac{1}{n}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(2^c\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2\gamma_j\zeta(\alpha)\right)\right) \\ &\le \frac{1}{n}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left(\prod_{j\notin\mathfrak{u}}\beta_j\prod_{j\in\mathfrak{u}}\left(2^{c+1}\gamma_j\zeta(\alpha)\right)\right) \\ &= \frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right) - \prod_{j=1}^{d}\beta_j\right) \\ &\le \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right). \end{aligned}$$

This completes the proof. □

Corollary 5.6 [cf. Corollary 3.7] *There exists a choice of* $\boldsymbol{z} \in \mathcal{Z}_n^d$ *such that*

$$e_{n,d}^2(\boldsymbol{z}) \leq \min\left(\frac{1}{\phi(n)} \prod_{j=1}^{d} \left(\beta_j + 2\gamma_j \zeta(\alpha)\right), \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + 2^{c+1}\gamma_j \zeta(\alpha)\right) \right),$$

where c *is the number of distinct prime factors of* n.

Though this second bound is generally larger than the first bound (but not always as is shown by the case $d = 1$ and $n = 2^q$ for $q \geq 1$), and seems to be of no apparent use, it will be required later on when we consider the component-by-component construction of the generating vector $\boldsymbol{z}$.

Let us now consider the set of integers n whose number of distinct prime factors is bounded by a constant, that is, we assume that $c \leq c_{\max} < \infty$, where $c_{\max}$ is some chosen value. Thus

$$\frac{n}{\phi(n)} \leq 2^c \leq 2^{c_{\max}} < \infty.$$

The bounds from Corollary 5.6 are clearly of the form given in Theorem 2.9 (with either $a = 2\zeta(\alpha)$ and $b = \frac{n}{\phi(n)}$ or $a = 2^{c+1}\zeta(\alpha)$ and $b = 1$). We thus conclude that *the family of rank-1 lattice rules with a composite number of points is strongly tractable in weighted Korobov spaces if and only if*

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty.$$

5.1.3 Component-by-component construction for general n

Theorem 5.8 below gives the theoretical foundation for the component-by-component construction when n is a composite number. The proof of Theorem 5.8 makes use of the following result which is very similar to Lemma 5.4.

Lemma 5.7 [cf. Lemma 5.4] *Let* $S_\alpha(k, n)$ *be as given in Definition 5.1. Then*

$$\sum_{k=1}^{n} |S_\alpha(k, n)| \leq 2^c,$$

where c *is the number of distinct prime factors of* n.

Proof. Given $\alpha > 1$, let

$$\tilde{F}_\alpha(n) := \sum_{k=1}^{n} |S_\alpha(k,n)|.$$

Using a similar argument as in the proof of Lemma 5.4, we deduce that $\tilde{F}_\alpha$ is a multiplicative arithmetic function and thus for $n = p_1^{q_1} p_2^{q_2} \cdots p_c^{q_c}$, where $p_1, \ldots, p_c$ are distinct primes, we have

$$\tilde{F}_\alpha(n) = \prod_{t=1}^{c} \tilde{F}_\alpha(p_t^{q_t})$$

For p a prime number and $q \geq 1$, we have from the proof of Lemma 5.4 that

$$S_\alpha(k, p^q) = \frac{1}{p^{\alpha q - 1}(p-1)} J(k),$$

where

$$J(k) = \begin{cases} p^{\alpha q - 1}(p-1), & \text{if } k = p^q, \\ 1 - p^{\alpha - 1}, & \text{if } \gcd(p^q, k) = 1, \\ p^{\alpha i}(1 - p^{\alpha - 1}), & \text{if } \gcd(p^q, k) = p^i,\ 1 \leq i \leq q-1. \end{cases}$$

Thus

$$\begin{aligned} \tilde{F}_\alpha(p^q) &= \sum_{k=1}^{p^q} |S_\alpha(k, p^q)| \\ &= \frac{1}{p^{\alpha q - 1}(p-1)} \sum_{k=1}^{p^q} |J(k)| \\ &= \frac{1}{p^{\alpha q - 1}(p-1)} \left(|J(p^q)| + \sum_{\substack{k=1 \\ \gcd(p^q,k)=1}}^{p^q} |J(k)| + \sum_{i=1}^{q-1} \sum_{\substack{k=1 \\ \gcd(p^q,k)=p^i}}^{p^q} |J(k)| \right), \end{aligned}$$

Now $|J(p^q)| = p^{\alpha q - 1}(p-1)$ and

$$\begin{aligned} \sum_{\substack{k=1 \\ \gcd(p^q,k)=1}}^{p^q} |J(k)| &= \sum_{\substack{k=1 \\ \gcd(p^q,k)=1}}^{p^q} \left|1 - p^{\alpha-1}\right| \\ &= \left(p^q - p^{q-1}\right)\left(p^{\alpha-1} - 1\right) \\ &= p^{q-1}(p-1)\left(p^{\alpha-1} - 1\right), \end{aligned}$$

while

$$\begin{aligned}
\sum_{i=1}^{q-1} \sum_{\substack{k=1 \\ \gcd(p^q,k)=p^i}}^{p^q} |J(k)| &= \sum_{i=1}^{q-1} \sum_{\substack{k=1 \\ \gcd(p^q,k)=p^i}}^{p^q} \left|p^{\alpha i}(1-p^{\alpha-1})\right| \\
&= \sum_{i=1}^{q-1}(p^{q-i}-p^{q-i-1})p^{\alpha i}(p^{\alpha-1}-1) \\
&= p^{q-1}(p-1)(p^{\alpha-1}-1)\sum_{i=1}^{q-1}(p^{\alpha-1})^i \\
&= p^{q-1}(p-1)(p^{\alpha-1}-1)\frac{p^{(\alpha-1)q}-p^{\alpha-1}}{p^{\alpha-1}-1}.
\end{aligned}$$

Upon combining these expressions together and doing some algebraic manipulations, we obtain

$$\begin{aligned}
\tilde{F}_\alpha(p^q) &= \frac{1}{p^{(\alpha q-1)}(p-1)}\Bigg[p^{(\alpha q-1)}(p-1)+p^{q-1}(p-1)(p^{\alpha-1}-1) \\
&\qquad +p^{q-1}(p-1)(p^{\alpha-1}-1)\frac{p^{(\alpha-1)q}-p^{\alpha-1}}{p^{\alpha-1}-1}\Bigg] \\
&= 2-\frac{1}{p^{(\alpha-1)q}} \le 2.
\end{aligned}$$

Hence

$$\tilde{F}_\alpha(n) = \prod_{t=1}^{c} \tilde{F}_\alpha(p_t^{q_t}) \le \prod_{t=1}^{c} 2 \le 2^c.$$

This completes the proof. We see from the exact expression for $\tilde{F}_\alpha(p^q)$ given above that this bound on $\tilde{F}_\alpha(n)$ cannot be significantly improved. □

As in Chapter 3, $e_{n,d}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1})$ denotes the worst-case error for a QMC rule with the set of points $\{\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}\}$, and $e_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ denotes the worst-case error for a QMC rule with the set of points

$$\left\{\left(\boldsymbol{x}_i,\left\{\frac{iz_{d+1}}{n}\right\}\right) : 0 \le i \le n-1\right\}.$$

Theorem 5.8 [cf. Theorem 3.8] *Suppose there exist $\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1} \in [0,1]^d$ such that*

$$e_{n,d}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \le \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+2^{c+1}\gamma_j\zeta(\alpha)\right),$$

where c is the number of distinct prime factors of n. Then there exists $z_{d+1} \in \mathcal{Z}_n$ such that

$$e_{n,d+1}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}) \le \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j+2^{c+1}\gamma_j\zeta(\alpha)\right).$$

Such a z_{d+1} *can be found by minimizing* $e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ *over the set* $\mathcal{Z}_n$.

Proof. Suppose that $\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}$ satisfy the assumed bound, and let

$$m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) := \frac{1}{\phi(n)} \sum_{z_{d+1}\in\mathcal{Z}_n} e^2_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}).$$

Following the proof of Theorem 3.8, we see that the result is proved if we can prove that

$$m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \le \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right).$$

We see from the proof of Theorem 3.8 that

$$\begin{aligned} & m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ \le\; & \beta_{d+1}e^2_{n,d}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) + \frac{\gamma_{d+1}}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|\tilde{T}_\alpha(i-k,n)|\prod_{j=1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right), \end{aligned}$$

where

$$\tilde{T}_\alpha(k,n) := \frac{1}{\phi(n)}\sum_{\substack{z=1\\ \gcd(z,n)=1}}^{n-1}\ \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i hkz/n}}{|h|^\alpha}. \tag{5.1}$$

Note that $\tilde{T}_\alpha(n,n) = \tilde{T}_\alpha(0,n)$, $\tilde{T}_\alpha(k,n) = \tilde{T}_\alpha(k \bmod n, n)$, and we see from Lemma 5.2 that $\tilde{T}_\alpha(k,n) = 2\zeta(\alpha)S_\alpha(k,n)$ if $1 \le k \le n$. (Also if n is a prime number, $\tilde{T}_\alpha(k,n)$ is exactly $T_\alpha(k,n)$ as given in Lemma 3.2.) Now since for $0 \le i,k \le n-1$, the values of $(i-k) \bmod n$ are just 0 to $n-1$ in some order each occurring n times, we have

$$\begin{aligned} \sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|\tilde{T}_\alpha(i-k,n)| &= \sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|\tilde{T}_\alpha((i-k) \bmod n,n)| \\ &= n\sum_{k=0}^{n-1}|\tilde{T}_\alpha(k,n)| \\ &= n\sum_{k=1}^{n}|\tilde{T}_\alpha(k,n)| \\ &= n\sum_{k=1}^{n}|2\zeta(\alpha)S_\alpha(k,n)| \\ &= 2\zeta(\alpha)n\sum_{k=1}^{n}|S_\alpha(k,n)| \le 2^{c+1}\zeta(\alpha)n, \end{aligned} \tag{5.2}$$

where we have used Lemma 5.7. Hence

$$\begin{aligned} & m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ \leq\ & \frac{\beta_{d+1}}{n}\prod_{j=1}^{d}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right) + \frac{2^{c+1}\gamma_{d+1}\zeta(\alpha)}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) \\ \leq\ & \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right). \end{aligned}$$

This completes the proof. □

Corollary 5.9 [cf. Corollary 3.9] *We can construct $\boldsymbol{z} \in \mathcal{Z}_n^d$ component-by-component such that for all $s = 1, \ldots, d$,*

$$e_{n,s}^2(z_1,\ldots,z_s) \leq \frac{1}{n}\prod_{j=1}^{s}\left(\beta_j + 2^{c+1}\gamma_j\zeta(\alpha)\right).$$

We can set $z_1 = 1$, and for s satisfying $2 \leq s \leq d$, each z_s can be found by minimizing $e_{n,s}^2(z_1,\ldots,z_s)$ over the set $\mathcal{Z}_n$.

Proof. Following the proof of Corollary 3.9, we see that the result is proved if we can prove that

$$e_{n,1}^2(1) \leq \frac{1}{n}\left(\beta_1 + 2^{c+1}\gamma_1\zeta(\alpha)\right).$$

This is clearly true since we have from (3.2) that $e_{n,1}^2(1) = \frac{2\gamma_1\zeta(\alpha)}{n^\alpha}$. □

For the set of integers n whose number of distinct prime factors, c, is bounded by a constant, Corollary 5.9 leads us to the following algorithm for constructing rank-1 lattice rules that achieve strong tractability error bounds given in Theorem 2.9 with $a = 2^{c+1}$ and $b = 1$.

Algorithm 5.10 [cf. Algorithm 3.10]

1. *Set z_1, the first component of $\boldsymbol{z}$, to* 1.

2. *For $s = 2, 3, \ldots, d-1, d$, find $z_s \in \mathcal{Z}_n = \{1 \leq z \leq n-1 : \gcd(z, n) = 1\}$ such that*

$$e_{n,s}^2(z_1,\ldots,z_s) = -\prod_{j=1}^{s}\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}\frac{e^{2\pi i hkz_j/n}}{|h|^\alpha}\right)$$

is minimized.

The cost of constructing a n-point rank-1 lattice rule up to d dimensions is approximately $O(n\phi(n)d^2)$ operations. This can be reduced to $O(n\phi(n)d)$ operations if we store the products during the search, but this would be at the expense of $O(n)$ storage.

5.2 Shifted rank-1 lattice rules in weighted Sobolev spaces

Now we generalize the results from Chapter 4 to shifted rank-1 lattice rules with a composite number of points in weighted Sobolev spaces. As in Chapter 4, we exploit the relationship of the worst-case errors between weighted Sobolev spaces and weighted Korobov spaces.

5.2.1 Mean and upper bound for general n

With the same arguments as those in the proof of Theorem 4.2, we obtain the following result using Theorems 5.3 and 5.5.

Theorem 5.11 [cf. Theorem 4.2] *We have*

$$M_{n,d} = -\prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{3}\right) + \frac{1}{n}\sum_{k=1}^{n}\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(\frac{1}{3} + \frac{S_2(k,n)}{6}\right)\right),$$

where $S_2(k,n)$ is as given in Definition 5.1 with $\alpha = 2$. Moreover,

$$M_{n,d} \leq \min\left(\frac{1}{\phi(n)}\prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{2}\right), \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right)\right).$$

Corollary 5.12 [cf. Corollary 4.3] *There exist a choice of $\boldsymbol{z} \in \mathcal{Z}_n^d$ and a choice of $\boldsymbol{\Delta} \in [0,1)^d$ such that*

$$e_{n,d}^2(\boldsymbol{z},\boldsymbol{\Delta}) \leq \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right),$$

where c is the number of distinct prime factors of n.

We then conclude from the above corollary and Theorem 2.9 that *the family of shifted rank-1 lattice rules with a composite number of points is strongly tractable in weighted Sobolev spaces if and only if*

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty.$$

5.2.2 Component-by-component construction for general n

As in Chapter 4, we will let $e_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$ denote the worst-case error for a QMC rule with the set of points

$$\left\{ \left(\boldsymbol{x}_i, \left\{ \frac{iz_{d+1}}{n} + \Delta_{d+1} \right\} \right) : 0 \le i \le n-1 \right\}.$$

Theorem 5.13 below, which generalizes Theorem 4.6, gives the theoretical foundation for the component-by-component construction when n is a composite number.

Theorem 5.13 [cf. Theorem 4.6] *Suppose there exist $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1} \in [0,1]^d$ such that*

$$e^2_{n,d}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \le \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \frac{2^c+1}{3} \gamma_j \right),$$

where c is the number of distinct prime factors of n. Then there exist $z_{d+1} \in \mathcal{Z}_n$ and $\Delta_{d+1} \in [0,1)$ such that

$$e^2_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1}) \le \frac{1}{n} \prod_{j=1}^{d+1} \left(\beta_j + \frac{2^c+1}{3} \gamma_j \right).$$

A pair (z_{d+1}, Δ_{d+1}) satisfying this bound can be found by first finding a $z_{d+1} \in \left\{1 \le z \le \frac{n-1}{2} : \gcd(z,n) = 1\right\}$ that minimizes $\omega_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$ and then (with this z_{d+1} fixed) finding a $\Delta_{d+1} \in \left\{\frac{2m-1}{2n} : m = 1, \ldots, n\right\}$ that minimizes $e^2_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$.

Proof. Suppose that $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ satisfy the assumed bound, and let

$$m_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) := \frac{1}{n-1} \sum_{z_{d+1} \in \mathcal{Z}_n} \omega_{n,d+1}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}),$$

where $\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1})$ is as given in Lemma 4.4. Following the proof of Theorem 4.6, we see that the result is proved if we can prove that

$$m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \le \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right).$$

We see from the proof of Theorem 4.6 that

$$\begin{aligned} m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \;\le\; & \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) e_{n,d}^2(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ & + \frac{\gamma_{d+1}}{2\pi^2 n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|\tilde{T}_2(i-k,n)|\prod_{j=1}^{d}(\beta_j+\gamma_j), \end{aligned}$$

where

$$\tilde{T}_2(k,n) := \frac{1}{\phi(n)}\sum_{\substack{z=1\\ \gcd(z,n)=1}}^{n-1}\;\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z/n}}{h^2}$$

is exactly the expression (5.1) with $\alpha = 2$. It then follows from (5.2) that

$$\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|\tilde{T}_2(i-k,n)| \le 2^{c+1}\zeta(2)n = \frac{2^c\pi^2 n}{3}.$$

Thus

$$\begin{aligned} & m_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ \le\; & \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right)\times\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right) + \frac{2^{c-1}\gamma_{d+1}}{3n}\prod_{j=1}^{d}(\beta_j+\gamma_j) \\ \le\; & \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right). \end{aligned}$$

By the symmetric property of B_2, we see that

$$\omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}) = \omega_{n,d+1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};n-z_{d+1}).$$

Also, if $\gcd(z_{d+1},n) = 1$, then $\gcd(n-z_{d+1},n) = 1$. Thus the search of z_{d+1} can be restricted to the set $\left\{1 \le z \le \frac{n-1}{2} : \gcd(z,n) = 1\right\}$. This completes the proof. □

Corollary 5.14 [cf. Corollary 4.7] *We can construct* $\boldsymbol{z} \in \mathcal{Z}_n^d$ *and* $\boldsymbol{\Delta} \in [0,1)^d$ *component-by-component such that for all* $s = 1,\ldots,d$,

$$e_{n,s}^2\left((z_1,\ldots,z_s),(\Delta_1,\ldots,\Delta_s)\right) \le \frac{1}{n}\prod_{j=1}^{s}\left(\beta_j + \frac{2^c+1}{3}\gamma_j\right).$$

We can set $z_1 = 1$, *and find* Δ_1 *in the set* $\left\{\frac{2m-1}{2n} : m = 1, \ldots, n\right\}$ *to minimize* $e_{n,1}^2(1, \Delta_1)$. *For* s *satisfying* $2 \leq s \leq d$, *each pair* (z_s, Δ_s) *can be found by first finding a* z_s *in* $\left\{1 \leq z \leq \frac{n-1}{2} : \gcd(z, n) = 1\right\}$ *that minimizes*

$$\begin{aligned}
&\omega_{n,s}\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1}); z_s\right) \\
&= \left(\beta_s + \frac{\gamma_s}{3}\right) e_{n,s-1}^2\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1})\right) \\
&\quad + \frac{\gamma_s}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{s-1} \left(\beta_j + \gamma_j \left[1 - \max\left(\left\{\frac{iz_j}{n} + \Delta_j\right\}, \left\{\frac{kz_j}{n} + \Delta_j\right\}\right)\right]\right)\right. \\
&\qquad \left. \times B_2\left(\left\{\frac{(i-k)z_s}{n}\right\}\right)\right],
\end{aligned}$$

and then (with this z_s *fixed) finding a* Δ_s *in* $\left\{\frac{2m-1}{2n} : m = 1, \ldots, n\right\}$ *that minimizes* $e_{n,s}^2\left((z_1, \ldots, z_s), (\Delta_1, \ldots, \Delta_s)\right)$.

Proof. Following the proof of Corollary 4.7, we see that the result is proved if we can prove that

$$\omega_{n,1}(1) \leq \frac{1}{n}\left(\beta_1 + \frac{2^c + 1}{3}\gamma_1\right).$$

This is clearly true since we have from (4.2) that $\omega_{n,1}(1) = \frac{\gamma_1}{6n^2}$. This completes the proof. □

For the set of integers n whose number of distinct prime factors, c, is bounded by a constant, Corollary 4.7 leads us to the following algorithm for constructing rank-1 lattice rules that achieve strong tractability error bounds given in Theorem 2.15 with $a = \frac{2^c+1}{3}$ and $b = 1$.

Algorithm 5.15 [cf. Algorithm 4.8]

1. *Set* z_1, *the first component of* $\boldsymbol{z}$, *to* 1.

2. *Find* $\Delta_1 \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ *to minimize*

$$\begin{aligned}
e_{n,1}^2(1, \Delta_1) &= \frac{\gamma_1}{3} + \frac{\gamma_1}{n}\left\{\frac{i}{n} + \Delta_1\right\}^2 \\
&\quad - \frac{\gamma_1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \max\left(\left\{\frac{i}{n} + \Delta_1\right\}, \left\{\frac{k}{n} + \Delta_1\right\}\right).
\end{aligned}$$

3. For $s = 2, 3, \ldots, d-1, d$, do the following:

(a) Find $z_s \in \left\{1 \le z \le \frac{n-1}{2} : \gcd(z,n) = 1\right\}$ to minimize

$$
\begin{aligned}
&\omega_{n,s}\left((z_1,\ldots,z_{s-1}),(\Delta_1,\ldots,\Delta_{s-1}),z_s\right) \\
&= \left(\beta_s + \frac{\gamma_s}{3}\right) e^2_{n,s-1}\left((z_1,\ldots,z_{s-1}),(\Delta_1,\ldots,\Delta_{s-1})\right) \\
&\quad + \frac{\gamma_s}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[1 - \max\left(\left\{\tfrac{iz_j}{n}+\Delta_j\right\},\left\{\tfrac{kz_j}{n}+\Delta_j\right\}\right)\right]\right)\right. \\
&\qquad\qquad \left. \times B_2\left(\left\{\tfrac{(i-k)z_s}{n}\right\}\right)\right]
\end{aligned}
$$

(b) Find $\Delta_s \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize

$$
\begin{aligned}
&e^2_{n,s}\left((z_1,\ldots,z_s),(\Delta_1,\ldots,\Delta_s)\right) \\
&= \prod_{j=1}^{s}\left(\beta_j + \frac{\gamma_j}{3}\right) - \frac{2}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left[\beta_j + \frac{\gamma_j}{2}\left(1 - \left\{\tfrac{iz_j}{n}+\Delta_j\right\}^2\right)\right] \\
&\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[\beta_j + \gamma_j\left(1 - \max\left(\left\{\tfrac{iz_j}{n}+\Delta_j\right\},\left\{\tfrac{kz_j}{n}+\Delta_j\right\}\right)\right)\right].
\end{aligned}
$$

The cost of constructing a rule for all dimensions up to d is approximately $O(n^2\phi(n)d^2)$ operations, which can be reduced to $O(n^2\phi(n)d)$ operations at the expense of $O(n^2)$ storage.

Chapter 6

Constructing Randomly Shifted Rank-1 Lattice Rules in Weighted Sobolev Spaces

In the construction of shifted rank-1 lattice rules in Chapters 4 and 5, the shifts were generated in a deterministic manner. Here we propose the alternative of allowing the shifts to be random, opening the possibility of repeating the calculation with a number of independent shifts so as to allow error estimation. An important advantage of this is that the cost of the construction is reduced from $O(n^3d^2)$ operations to $O(n^2d^2)$ operations. We remark that when the sum of γ_j/β_j is finite, the rules thus constructed achieve a worst-case strong tractability error bound in a probabilistic sense: the mean square worst-case errors over all possible shifts satisfy the desired bound.

6.1 Randomly shifted rank-1 lattice rules

Randomly shifted rank-1 lattice rules are, as the name suggested, shifted rank-1 lattice rules in which the shifts are chosen randomly. The underlying idea is not new. For example, as early as 1976 Cranley and Patterson [5] pointed out the benefits of using random shifts with rank-1 lattice rules; later this idea was generalized to other lattice rules by Joe [14]. Later still, Owen in [26] introduced a similar randomization idea ('scrambled (t, m, d)-nets') into nets. By now the idea of combining randomization (or 'Monte Carlo') ideas with deterministic QMC ideas is commonplace. The key underlying concepts behind such randomized QMC methods are discussed in [10].

Let q be a positive integer, and let $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{q-1}$ be q independent random shifts drawn from a uniform distribution on $[0,1]^d$. We can obtain an approximation based on the average:

$$\bar{Q}_{n,d}(f) := \frac{1}{qn} \sum_{m=0}^{q-1} \sum_{i=0}^{n-1} f\left(\left\{\frac{i\boldsymbol{z}}{n} + \boldsymbol{\Delta}_m\right\}\right), \tag{6.1}$$

where $\boldsymbol{z} \in \mathcal{Z}_n^d$ is the generating vector.

6.1.1 An unbiased estimator

We show that the approximation $\bar{Q}_{n,d}(f)$ is an unbiased estimator of $I_d(f)$. Since this result is true not only for rank-1 lattice rules but also for all equal-weight quadrature rules, we state the result in its general form.

Let $Q_{n,d}(f)$ be an n-point equal-weight quadrature rule with quadrature points $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1} \in [0,1]^d$, and for $\boldsymbol{\Delta} \in [0,1]^d$, let $Q_{n,d}(f; \boldsymbol{\Delta})$ denote the associated $\boldsymbol{\Delta}$-shifted rule:

$$Q_{n,d}(f; \boldsymbol{\Delta}) := \frac{1}{n} \sum_{i=0}^{n-1} f(\{\boldsymbol{x}_i + \boldsymbol{\Delta}\}).$$

For q a positive integer and $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{q-1} \in [0,1]^d$, let $\bar{Q}_{n,d}(f; \boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{q-1})$ denote the approximation obtained by taking an average over q random shifts, that is,

$$\bar{Q}_{n,d}(f; \boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{q-1}) := \frac{1}{q} \sum_{m=0}^{q-1} Q_{n,d}(f; \boldsymbol{\Delta}_m) = \frac{1}{qn} \sum_{m=0}^{q-1} \sum_{i=0}^{n-1} f(\{\boldsymbol{x}_i + \boldsymbol{\Delta}_m\}),$$

where $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{q-1}$ are independent random vectors having a uniform distribution on $[0,1]^d$.

Theorem 6.1 *The family of shifted rules $Q_{n,d}(f;\boldsymbol{\Delta})$ is an unbiased estimator of the integral $I_d(f)$, in the sense that*

$$\mathcal{E}\left[Q_{n,d}(f;\cdot)\right] := \int_{[0,1]^d} Q_{n,d}(f;\boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta} = I_d(f).$$

Proof. We have

$$\mathcal{E}\left[Q_{n,d}(f;\cdot)\right] = \frac{1}{n}\sum_{i=0}^{n-1}\int_{[0,1]^d} f(\{\boldsymbol{x}_i+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta} = \frac{1}{n}\sum_{i=0}^{n-1}\int_{[0,1]^d} f(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = I_d(f),$$

where in the second to last step we have made a change of variable. □

Corollary 6.2 *The mean $\bar{Q}_{n,d}(f;\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1})$ is an unbiased estimate of $I_d(f)$, and has variance*

$$\sigma^2 = \frac{1}{q}\mathcal{E}\left[\left(Q_{n,d}(f;\cdot) - I_d(f)\right)^2\right] = \frac{1}{q}\int_{[0,1]^d}\left(Q_{n,d}(f;\boldsymbol{\Delta}) - I_d(f)\right)^2\mathrm{d}\boldsymbol{\Delta}.$$

Proof. See Corollary 3 of [14]. □

It is well-known that an unbiased estimate of σ, the standard error of the mean $\bar{Q}_{n,d}(f;\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1})$, is

$$\tilde{\sigma} := \left(\frac{1}{q(q-1)}\sum_{m=0}^{q-1}\left[Q_{n,d}(f;\boldsymbol{\Delta}_m) - \bar{Q}_{n,d}(f;\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1})\right]^2\right)^{1/2}$$

By using the well-known Chebyshev inequality (see [21]),

$$\text{probability}\left(\left|\bar{Q}_{n,d}(f;\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}) - I_d(f)\right| < k\sigma\right) \geq 1 - \frac{1}{k^2},$$

this estimate of σ allows us to calculate confidence intervals for the error, that is, an interval in which the true error must lie with a fixed probability.

Since the theorem and the corollary hold for any equal-weight quadrature rule $Q_{n,d}(f)$, then it certainly holds for rank-1 lattice rules, thus the average (6.1) is an unbiased estimate of the integral $I_d(f)$.

6.1.2 Expected value of square worst-case error

Let $P_{n,d} = \{\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}\}$ and $P_{n,d}(\boldsymbol{\Delta}) = \{\{\boldsymbol{x}_i+\boldsymbol{\Delta}\} : 0 \leq i \leq n-1\}$ denote the sets of quadrature points for a QMC rule $Q_{n,d}(f)$ and its associated Δ-shifted rule $Q_{n,d}(f;\boldsymbol{\Delta})$. Since the mean $\bar{Q}_{n,d}(f;\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1})$ can be considered as an equal-weight quadrature rule with qn points, we denote its set of quadrature points by

$$P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}) = \{\{\boldsymbol{x}_i+\boldsymbol{\Delta}_m\} : 0\le i\le n-1,\, 0\le m\le q-1\}.$$

Now suppose that f belongs to a certain reproducing kernel Hilbert space with kernel K_d, and suppose K_d^* is the shift-invariant kernel associated with K_d (see (2.4)). Since the shifts are to be chosen randomly, we consider the expected value

$$\begin{aligned}&\mathcal{E}\left[e^2_{q,n,d}\left(P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}),K_d\right)\right]\\ &:= \int_{[0,1]^{qd}} e^2_{q,n,d}\left(P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}),K_d\right)\,\mathrm{d}\boldsymbol{\Delta}_0\cdots\mathrm{d}\boldsymbol{\Delta}_{q-1}.\end{aligned}$$

In the special case of $q=1$, we know from Lemma 2.4 that

$$\mathcal{E}\left[e^2_{n,d}\left(P_{n,d}(\boldsymbol{\Delta}),K_d\right)\right] := \int_{[0,1]^d} e^2_{n,d}\left(P_{n,d}(\boldsymbol{\Delta}),K_d\right)\,\mathrm{d}\boldsymbol{\Delta} = e^2_{n,d}(P_{n,d},K_d^*),$$

that is, the expected value of the square worst-case error for the shifted rule in the Hilbert space with reproducing kernel K_d is exactly the same as the square worst-case error for the original unshifted rule in the Hilbert space with reproducing kernel K_d^*.

We now obtain a similar result for $\mathcal{E}\left[e^2_{q,n,d}\left(P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}),K_d\right)\right]$, and we would expect the result to match the above when $q=1$.

Theorem 6.3 *We have*

$$\mathcal{E}\left[e^2_{q,n,d}\left(P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}),K_d\right)\right] = \frac{1}{q}e^2_{n,d}(P_{n,d},K_d^*).$$

Proof. We see from a slight generalization of Lemma 2.2 that

$$\begin{aligned}&e^2_{q,n,d}\left(P_{q,n,d}(\boldsymbol{\Delta}_0,\ldots,\boldsymbol{\Delta}_{q-1}),K_d\right)\\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{qn}\sum_{m=0}^{q-1}\sum_{i=0}^{n-1}\int_{[0,1]^d} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}_m\},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\\ &\quad+\frac{1}{q^2n^2}\sum_{m=0}^{q-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}_m\},\{\boldsymbol{x}_k+\boldsymbol{\Delta}_m\})\\ &\quad+\frac{1}{q^2n^2}\sum_{m=0}^{q-1}\sum_{\substack{\ell=0\\ \ell\ne m}}^{q-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\{\boldsymbol{x}_i+\boldsymbol{\Delta}_m\},\{\boldsymbol{x}_k+\boldsymbol{\Delta}_\ell\}).\end{aligned}$$

Thus we have

$$
\begin{aligned}
&\mathcal{E}\left[e^2_{q,n,d}\left(P_{q,n,d}(\mathbf{\Delta}_0,\ldots,\mathbf{\Delta}_{q-1}),K_d\right)\right]\\
&= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{qn}\sum_{m=0}^{q-1}\sum_{i=0}^{n-1}\int_{[0,1]^{2d}} K_d(\{\boldsymbol{x}_i+\mathbf{\Delta}_m\},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\mathbf{\Delta}_m\\
&\quad+\frac{1}{q^2n^2}\sum_{m=0}^{q-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^{d}} K_d(\{\boldsymbol{x}_i+\mathbf{\Delta}_m\},\{\boldsymbol{x}_k+\mathbf{\Delta}_m\})\,\mathrm{d}\mathbf{\Delta}_m\\
&\quad+\frac{1}{q^2n^2}\sum_{m=0}^{q-1}\sum_{\substack{\ell=0\\ \ell\neq m}}^{q-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^{2d}} K_d(\{\boldsymbol{x}_i+\mathbf{\Delta}_m\},\{\boldsymbol{x}_k+\mathbf{\Delta}_\ell\})\,\mathrm{d}\mathbf{\Delta}_m\,\mathrm{d}\mathbf{\Delta}_\ell,\\
&= \int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - 2\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\\
&\quad+\frac{1}{qn^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^{d}} K_d(\{\boldsymbol{x}_i+\mathbf{\Delta}\},\{\boldsymbol{x}_k+\mathbf{\Delta}\})\,\mathrm{d}\mathbf{\Delta}\\
&\quad+\frac{q-1}{q}\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\\
&= \frac{1}{q}\left(-\int_{[0,1]^{2d}} K_d(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\right.\\
&\qquad\left.+\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\int_{[0,1]^{d}} K_d(\{\boldsymbol{x}_i+\mathbf{\Delta}\},\{\boldsymbol{x}_k+\mathbf{\Delta}\})\,\mathrm{d}\mathbf{\Delta}\right).
\end{aligned}
$$

We see from the proof of Lemma 2.4 that the expression inside the brackets is $e^2_{n,d}(P_{n,d},K^*_d)$. This completes the proof. □

We then see that $\mathcal{E}\left[e^2_{q,n,d}\left(P_{q,n,d}(\mathbf{\Delta}_0,\ldots,\mathbf{\Delta}_{q-1}),K_d\right)\right]$ may be calculated by using $e^2_{n,d}(P_{n,d},K^*_d)$.

6.2 Component-by-component construction

So far we have looked at the general theory, and have not specified the rule or the reproducing kernel Hilbert space. Let $K_d = K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ be a kernel for some weighted Sobolev space (see (2.11)), and let $\bar{Q}_{n,d}(f)$ be the mean given by (6.1), that is, the average of q randomly shifted rank-1 lattice rules.

Let $K^*_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ denote the shift-invariant kernel associated with $K_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$, and let $\hat{e}_{n,d}(\boldsymbol{z})$ denote the worst-case error for a rank-1 lattice rule with generating vector $\boldsymbol{z}$ in the space with kernel $K^*_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$. From the preceding discussion, it is clear that if we wish to use random shifts of rank-1 lattice rules to estimate the integral $I_d(f)$, then we should choose rank-1 lattice rules which give the best value of $\hat{e}_{n,d}(\boldsymbol{z})$. Furthermore, to show that a rule of the form (6.1) achieves strongly tractability error bounds in a probabilistic sense, we need to show that $\hat{e}^2_{n,d}(\boldsymbol{z})$ satisfies a corresponding bound.

6.2.1 The known results

We see from Lemma 2.12 that $K^*_{d,\boldsymbol{\beta},\boldsymbol{\gamma}}$ is a kernel for some weighted Korobov space with parameters $\alpha = 2$,

$$\hat{\beta}_j = \beta_j + \frac{\gamma_j}{3} \quad \text{and} \quad \hat{\gamma}_j = \frac{\gamma_j}{2\pi^2}.$$

Thus it follows from Lemma 3.1 with these change of parameters and (2.8) that

$$\hat{e}^2_{n,d}(\boldsymbol{z}) = -\prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{3}\right) + \frac{1}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right) + \frac{1}{3}\right]\right), \quad (6.2)$$

where $B_2(x) = x^2 - x + \frac{1}{6}$ is the second degree Bernoulli polynomial.

When n is a prime number, it follows from Corollary 3.7 with these change of parameters that there exists a choice of $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that

$$\hat{e}^2_{n,d}(\boldsymbol{z}) \leq \min\left(\frac{2}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{2}\right), \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \frac{2\gamma_j}{3}\right)\right).$$

Moreover, it follows from Corollary 3.9 with the same change of parameters that if we set $z_1 = 1$ and find each $z_s \in \mathbb{Z}_n$ for $s = 2, \ldots, d$ by minimizing $\hat{e}^2_{n,s}(z_1, \ldots, z_s)$, then

$$\hat{e}^2_{n,s}(z_1, \ldots, z_s) \leq \frac{1}{n}\prod_{j=1}^{s}\left(\beta_j + \frac{2\gamma_j}{3}\right).$$

is satisfied for all $s = 1, \ldots, d$. We see from Theorem 2.15 that these bounds are clearly sufficient for strong tractability in weighted Sobolev spaces.

For general n, we can obtain similar results with bounds dependent on c, the number of distinct prime factors of n, using Corollary 5.6 and Corollary 5.9. If we assume that c is no more than a constant $c_{\max} < \infty$, then the bounds are also sufficient for strong tractability. By the symmetric property of B_2, we see that $\hat{e}^2_{n,s}(z_1,\ldots,z_s) = \hat{e}^2_{n,s}(z_1,\ldots,n-z_s)$. Also, if $\gcd(z_s,n) = 1$ then $\gcd(n-z_s,n) = 1$. Thus the search for z_s can be restricted to the set $\{1 \le z \le \frac{n-1}{2} : \gcd(z,n) = 1\}$. We give the algorithm below for general n.

Algorithm 6.4

1. *Set* z_1*, the first component of* $\boldsymbol{z}$*, to* 1.

2. *For* $s = 2,3,\ldots,d-1,d$*, find* $z_s \in \{1 \le z \le \frac{n-1}{2} : \gcd(z,n) = 1\}$ *such that*

$$\hat{e}^2_{n,s}(z_1,\ldots,z_s) = -\prod_{j=1}^{s}\left(\beta_j + \frac{\gamma_j}{3}\right) + \frac{1}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right) + \frac{1}{3}\right]\right),$$

is minimized.

The cost of constructing $\boldsymbol{z}$ for for all dimensions up to d is $O(n^2d^2)$ operations, which can be reduced to $O(n^2d)$ at the expense of $O(n)$ storage.

6.2.2 An improved bound for the construction

Here we give a different upper bound for the construction when n is a prime number. We show that the rule constructed has a square worst-case error smaller than the QMC mean (see Lemma 2.17).

Theorem 6.5 *Let n be a prime number. Suppose there exists $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that*

$$\hat{e}^2_{n,d}(\boldsymbol{z}) \le E_{n,d}, \text{ where } E_{n,d} = \frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{2}\right) - \prod_{j=1}^{d}\left(\beta_j + \frac{\gamma_j}{3}\right)\right)$$

is the QMC mean. Then there exists $z_{d+1} \in \mathbb{Z}_n$ such that

$$\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \le E_{n,d+1}.$$

Such a z_{d+1} can be found by minimizing $\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over the set $\{1,2,\ldots,\frac{n-1}{2}\}$. Moreover, we have $\hat{e}^2_{n,1}(z_1) \le E_{n,1}$ for all $z_1 \in \mathbb{Z}_n$.

Proof. Suppose that $\boldsymbol{z}$ satisfies the assumed bound. For any $z_{d+1} \in \mathbb{Z}_n$, we have from (6.2) that

$$\begin{aligned}
&\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) \hat{e}^2_{n,d}(\boldsymbol{z}) \\
&\quad + \frac{\gamma_{d+1}}{n} \sum_{i=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right) + \frac{1}{3}\right]\right) B_2\left(\left\{\frac{iz_{d+1}}{n}\right\}\right)\right] \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) \hat{e}^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}}{6n} \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{2}\right) \\
&\quad + \frac{\gamma_{d+1}}{n} \sum_{i=1}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \left(B_2\left(\left\{\frac{iz_j}{n}\right\}\right) + \frac{1}{3}\right]\right) B_2\left(\left\{\frac{iz_{d+1}}{n}\right\}\right)\right),
\end{aligned}$$

where we have separated out the $i = 0$ term. Now we average this over all the possible values of z_{d+1} to form

$$\begin{aligned}
\hat{m}_{n,d+1}(\boldsymbol{z}) &:= \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} \hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right) \hat{e}^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}}{6n} \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{2}\right) + L(\boldsymbol{z}),
\end{aligned}$$

where

$$\begin{aligned}
L(\boldsymbol{z}) &= \frac{\gamma_{d+1}}{n} \sum_{i=1}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right) + \frac{1}{3}\right]\right) \right. \\
&\qquad \left. \times \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} B_2\left(\left\{\frac{iz_{d+1}}{n}\right\}\right)\right].
\end{aligned}$$

When n is prime, for fixed i satisfying $1 \le i \le n-1$ the values of $\left\{\frac{iz_{d+1}}{n}\right\}$ as z_{d+1} runs from 1 to $n-1$ are just $\frac{1}{n}, \frac{2}{n}, \ldots, \frac{n-1}{n}$ in some order, and hence we have

$$\begin{aligned}
\frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} B_2\left(\left\{\frac{iz_{d+1}}{n}\right\}\right) &= \frac{1}{n-1} \sum_{z=1}^{n-1} B_2\left(\frac{z}{n}\right) \\
&= \frac{1}{n-1} \left(\sum_{z=0}^{n-1} B_2\left(\frac{z}{n}\right) - B_2(0)\right) \\
&= \frac{1}{n-1} \left(\frac{1}{6n} - \frac{1}{6}\right) \\
&= -\frac{1}{6n}, \qquad (6.3)
\end{aligned}$$

where in the second to last step we have used (4.1). It then follows that

$$\begin{aligned} L(\boldsymbol{z}) &= -\frac{\gamma_{d+1}}{6n^2}\sum_{i=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right)+\frac{1}{3}\right]\right) \\ &= -\frac{\gamma_{d+1}}{6n}\left(\hat{e}^2_{n,d}(\boldsymbol{z})-\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right)+\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right)\right), \end{aligned}$$

where we have used the fact that, upon separating out the $i = 0$ term, $\hat{e}^2_{n,d}(\boldsymbol{z})$ from (6.2) can be written as

$$\begin{aligned} \hat{e}^2_{n,d}(\boldsymbol{z}) &= -\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right)+\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right) \\ &\quad +\frac{1}{n}\sum_{i=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\frac{iz_j}{n}\right\}\right)+\frac{1}{3}\right]\right). \end{aligned}$$

Thus

$$\begin{aligned} \hat{m}_{n,d+1}(\boldsymbol{z}) &= \left(\beta_{d+1}+\frac{\gamma_{d+1}}{3}\right)\hat{e}^2_{n,d}(\boldsymbol{z})+\frac{\gamma_{d+1}}{6n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right) \\ &\quad -\frac{\gamma_{d+1}}{6n}\left(\hat{e}^2_{n,d}(\boldsymbol{z})-\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right)+\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right)\right) \\ &= \left(\beta_{d+1}+\gamma_{d+1}\left(\frac{1}{3}-\frac{1}{6n}\right)\right)\hat{e}^2_{n,d}(\boldsymbol{z}) \\ &\quad +\gamma_{d+1}\left(\frac{1}{6n}+\frac{1}{6n^2}\right)\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right)-\frac{\gamma_{d+1}}{6n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right). \end{aligned}$$

Using the assumption of $\hat{e}^2_{n,d}(\boldsymbol{z}) \leq E_{n,d}$, we have

$$\begin{aligned} &\hat{m}_{n,d+1}(\boldsymbol{z}) \\ &\leq \left(\beta_{d+1}+\gamma_{d+1}\left(\frac{1}{3}-\frac{1}{6n}\right)\right)\times\frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right)-\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right)\right) \\ &\quad +\gamma_{d+1}\left(\frac{1}{6n}+\frac{1}{6n^2}\right)\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{2}\right)-\frac{\gamma_{d+1}}{6n}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right) \\ &= \frac{1}{n}\left(\prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{2}\right)-\prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{3}\right)\right)-\gamma_{d+1}\left(\frac{1}{6n}-\frac{1}{6n^2}\right)\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{3}\right) \\ &\leq \frac{1}{n}\left(\prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{2}\right)-\prod_{j=1}^{d+1}\left(\beta_j+\frac{\gamma_j}{3}\right)\right) \\ &= E_{n,d+1}. \end{aligned}$$

Now since $\hat{m}_{n,d+1}(\boldsymbol{z})$ is the average over all z_{d+1} of $\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$, if we choose $z_{d+1} \in \mathbb{Z}_n$ to minimize $\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$, then this choice of z_{d+1} will satisfy

$$\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \leq \hat{m}_{n,d+1}(\boldsymbol{z}) \leq E_{n,d+1}.$$

By the symmetric property of B_2, we have $\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) = \hat{e}^2_{n,d+1}(\boldsymbol{z}, n - z_{d+1})$. Thus the search of z_{d+1} can be restricted to the set $\left\{1, 2, \ldots, \frac{n-1}{2}\right\}$.

In one dimension, it is known that there is only one n-point lattice rule, namely, the n-point rectangle rule. Thus we may take $z_1 = 1$ and obtain from (6.2) that

$$\begin{aligned} \hat{e}^2_{n,1}(1) &= -\left(\beta_1 + \frac{\gamma_1}{3}\right) + \frac{1}{n}\sum_{i=0}^{n-1}\left(\beta_1 + \gamma_1\left[B_2\left(\frac{i}{n}\right) + \frac{1}{3}\right]\right) \\ &= \frac{\gamma_1}{n}\sum_{i=0}^{n-1} B_2\left(\frac{i}{n}\right) = \frac{\gamma_1}{6n^2}, \end{aligned}$$

where the last step follows from (4.1). Now since

$$E_{n,1} = \frac{1}{n}\left[\left(\beta_1 + \frac{\gamma_1}{2}\right) - \left(\beta_1 + \frac{\gamma_1}{3}\right)\right] = \frac{\gamma_1}{6n},$$

we have $\hat{e}^2_{n,1}(1) \leq E_{n,1}$. This completes the proof. □

Chapter 7

Constructing Intermediate-rank Lattice Rules

We have assumed that the weights $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ for weighted Korobov and weighted Sobolev spaces satisfy

$$\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots > 0.$$

This is to moderate the ordering of the coordinate directions so that the rate of change is greatest in the x_1 direction, not as great in the x_2 direction, and so on. The first few variables are thus in a sense more important than the rest and therefore it would seem intuitive to 'copy' the coordinates of the points a number of times in the first few dimensions. Here we propose to copy the points of a rank-1 lattice rule to yield an intermediate-rank lattice rule. We show that when the sum of γ_j/β_j is finite, the generating vector for the rule can also be constructed component-by-component to achieve strong tractability error bounds.

7.1 Intermediate-rank lattice rules in weighted Korobov spaces

In weighted Korobov spaces of periodic functions, we consider the (ℓ, r)-copy of a rank-1 lattice rule with generating vector $\boldsymbol{z}$, that is, an intermediate-rank lattice rule with $N = \ell^r n$ quadrature points given by the set (see (1.6))

$$\left\{ \left\{ \frac{i\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell} \right\} : 0 \leq i \leq n-1,\ 0 \leq m_1, \ldots, m_r \leq \ell - 1 \right\},$$

where $\ell \geq 1$, $\gcd(\ell, n) = 1$, and $0 \leq r \leq d$. When $r = 0$ and/or $\ell = 1$, we get just the original n-point rank-1 lattice rule. For $r \geq 1$, the resulting rule is a rank-r lattice rule. These intermediate-rank lattice rules have previously been considered in [15] and [17]. Typically, for reasons of tractability, we will take r to be a fixed number, say $r = 1$, 2, or 3. For the choice of ℓ it would seem reasonable on practical grounds and theoretical grounds (see Theorem 7.5 and Lemma 7.6) to take ℓ to be 2 in actual calculations. This value of $\ell = 2$ has been previously used in [15] and [17].

In this section, we shall see that the generating vectors constructed component-by-component satisfy strong tractability error bounds. Moreover, in certain circumstances, the intermediate-rank lattice rules constructed satisfy bounds which are better than the corresponding bounds for rank-1 lattice rules with approximately the same number of points.

For simplicity, we will assume again that n is a prime number. More general results can be obtained by emulating the more complicated analysis from Chapter 5.

7.1.1 Square worst-case error

Let $e_{n,d,copy(\ell,r)}(\boldsymbol{z})$ denote the worst-case error for our intermediate-rank lattice rule in weighted Korobov spaces. An expression for $e_{n,d,copy(\ell,r)}(\boldsymbol{z})$ is given in the next lemma. Note that though this intermediate-rank lattice rule has $N = \ell^r n$ points, the lemma shows that the worst-case error may be calculated by using a rule having just n points. We also remark that when $\ell = 1$ and/or $r = 0$, the result is the same as Lemma 3.1.

Lemma 7.1 [cf. Lemma 3.1] *We have*

$$\begin{aligned} e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}) &= -\prod_{j=1}^{d}\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\beta_j + \frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h\ell k z_j/n}}{|h|^\alpha}\right)\right. \\ &\qquad \left.\times \prod_{j=r+1}^{d}\left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z_j/n}}{|h|^\alpha}\right)\right]. \end{aligned}$$

Proof. We have from Lemma 2.7 that

$$\begin{aligned} & e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}) \\ &= -\prod_{j=1}^{d}\beta_j + \frac{1}{\ell^{2r}n^2}\sum_{q_r=0}^{\ell-1}\cdots\sum_{q_1=0}^{\ell-1}\sum_{m_r=0}^{\ell-1}\cdots\sum_{m_1=0}^{\ell-1}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} \\ &\qquad \left[\prod_{j=1}^{r}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h\left(\left\{\frac{iz_j}{n}+\frac{q_j}{\ell}\right\}-\left\{\frac{kz_j}{n}+\frac{m_j}{\ell}\right\}\right)}}{|h|^\alpha}\right)\right. \\ &\qquad \left.\times \prod_{j=r+1}^{d}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h\left(\left\{\frac{iz_j}{n}\right\}-\left\{\frac{kz_j}{n}\right\}\right)}}{|h|^\alpha}\right)\right]. \end{aligned}$$

This second term can be written as

$$\begin{aligned} &\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\frac{1}{\ell^2}\sum_{q=0}^{\ell-1}\sum_{m=0}^{\ell-1}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h((i-k)z_j/n+(q-m)/\ell)}}{|h|^\alpha}\right)\right)\right. \\ &\qquad \left.\times \prod_{j=r+1}^{d}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(i-k)z_j/n}}{|h|^\alpha}\right)\right]. \end{aligned} \tag{7.1}$$

For $0 \le q, m \le \ell - 1$, the values of $(q-m) \bmod \ell$ are just 0 to $\ell - 1$ in some order, with each value occurring ℓ times. Thus we have

$$\begin{aligned} &\frac{1}{\ell^2}\sum_{q=0}^{\ell-1}\sum_{m=0}^{\ell-1}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h((i-k)z_j/n+(q-m)/\ell)}}{|h|^\alpha}\right) \\ &= \frac{1}{\ell}\sum_{m=0}^{\ell-1}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h((i-k)z_j/n+m/\ell)}}{|h|^\alpha}\right). \end{aligned}$$

Now since

$$\sum_{m=0}^{\ell-1} e^{2\pi i h m/\ell} = \begin{cases} \ell, & \text{if } h \text{ is a multiple of } \ell, \\ 0, & \text{otherwise,} \end{cases}$$

we have

$$\begin{aligned}
\frac{1}{\ell}\sum_{m=0}^{\ell-1}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h((i-k)z_j/n+m/\ell)}}{|h|^\alpha}\right)
&= \beta_j+\frac{\gamma_j}{\ell}\sum_{h=-\infty}^{\infty}{}'\left(\frac{e^{2\pi i h(i-k)z_j/n}}{|h|^\alpha}\sum_{m=0}^{\ell-1}e^{2\pi i h m/\ell}\right)\\
&= \beta_j+\frac{\gamma_j}{\ell}\sum_{m=-\infty}^{\infty}{}'\left(\frac{e^{2\pi i m\ell(i-k)z_j/n}}{|m\ell|^\alpha}\times\ell\right)\\
&= \beta_j+\frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i h\ell(i-k)z_j/n}}{|h|^\alpha}.
\end{aligned}$$

Thus (7.1) can be simplified to

$$\frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\beta_j+\frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i h\ell(i-k)z_j/n}}{|h|^\alpha}\right)\times\prod_{j=r+1}^{d}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i h(i-k)z_j/n}}{|h|^\alpha}\right)\right],$$

which can be simplified even further to

$$\frac{1}{n}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\beta_j+\frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i h\ell k z_j/n}}{|h|^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j+\gamma_j\sum_{h=-\infty}^{\infty}{}'\frac{e^{2\pi i h k z_j/n}}{|h|^\alpha}\right)\right],$$

since for $0\le i,k\le n-1$, the values of $(i-k) \bmod n$ are just 0 to $n-1$ in some order, with each value occurring n times. This completes the proof. □

7.1.2 Mean and upper bound when n is prime

We define the mean of $e^2_{n,d,copy(\ell,r)}(\boldsymbol{z})$ over all values of $\boldsymbol{z}\in\mathbb{Z}_n^d$ for n prime by

$$M_{n,d,copy(\ell,r)} := \frac{1}{(n-1)^d}\sum_{\boldsymbol{z}\in\mathbb{Z}_n^d} e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}).$$

Theorem 7.2 below gives an explicit expression for this mean. Note that when $\ell=1$ and/or $r=0$, the result is the same as Theorem 3.3.

Theorem 7.2 [cf. Theorem 3.3] *Let n be a prime number. Then*

$$\begin{aligned}
M_{n,d,copy(\ell,r)} &= -\prod_{j=1}^{d}\beta_j+\frac{1}{n}\prod_{j=1}^{r}\left(\beta_j+\frac{2\gamma_j\zeta(\alpha)}{\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right)\\
&\quad+\frac{n-1}{n}\prod_{j=1}^{r}\left(\beta_j-\frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{(n-1)\ell^\alpha}\right)\\
&\qquad\times\prod_{j=r+1}^{d}\left(\beta_j-\frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right).
\end{aligned}$$

Proof. It follows from the expression for $e^2_{n,d,copy(\ell,r)}(\boldsymbol{z})$ in Lemma 7.1 that

$$M_{n,d,copy(\ell,r)} = -\prod_{j=1}^{d}\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\beta_j + \frac{\gamma_j}{\ell^\alpha}T_\alpha(\ell k, n)\right)\prod_{j=r+1}^{d}\left(\beta_j + \gamma_j T_\alpha(k,n)\right)\right],$$

where $T_\alpha(k,n)$ is as given in Lemma 3.2. Since $\ell \neq 0$ and $\gcd(\ell, n) = 1$, upon separating the $k = 0$ and $k \neq 0$ terms, the expression for the mean follows from Lemma 3.2. □

We now give an upper bound for the mean.

Theorem 7.3 [cf. Theorem 3.4] *Let n be a prime number such that $n \geq 1 + \frac{\gamma_1}{\beta_1}\zeta(\alpha)$. Then*

$$M_{n,d,copy(\ell,r)} \leq \frac{1}{n}\prod_{j=1}^{r}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right).$$

Proof. Since $\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots$, we have from the condition $n \geq 1 + \frac{\gamma_1}{\beta_1}\zeta(\alpha)$ that for all $j \geq 1$,

$$n \geq 1 + \frac{\gamma_j}{\beta_j}\zeta(\alpha),$$

which leads to

$$\frac{\gamma_j\zeta(\alpha)}{(n-1)\ell^\alpha} \leq \frac{\gamma_j\zeta(\alpha)}{n-1} \leq \beta_j.$$

Thus

$$\left|\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right| \leq \beta_j \quad \text{and} \quad \left|\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{(n-1)\ell^\alpha}\right| \leq \beta_j,$$

and this implies that

$$\prod_{j=1}^{r}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{(n-1)\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right) \leq \prod_{j=1}^{d}\beta_j.$$

Hence

$$M_{n,d,copy(\ell,r)} \leq \frac{1}{n}\prod_{j=1}^{r}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right),$$

which completes the proof. □

Clearly there must exist at least one vector $\boldsymbol{z}$ such that the square worst-case error is as good as the average.

Corollary 7.4 *Let n be a prime number such that $n \geq 1+\frac{\gamma_1}{\beta_1}\zeta(\alpha)$. Then there exists a choice of $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that*

$$\begin{aligned} e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}) &\leq \frac{1}{n}\prod_{j=1}^{r}\left(\beta_j + \frac{2\gamma_j\zeta(\alpha)}{\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) \\ &\leq \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right). \end{aligned}$$

Now let $N = \ell^r n$ denote the total number of quadrature points. It is obvious that the last bound given in Corollary 7.4 is of the form given in Theorem 2.9 with $a = 2\zeta(\alpha)$, $b = \ell^r$ and $n = N$. We thus conclude that *the family of intermediate-rank lattice rules (with n prime) is strongly tractable in weighted Korobov spaces if and only if*

$$\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty.$$

7.1.3 Comparison with rank-1 lattice rules

It follows from Theorem 7.2 with $\ell = 1$ and $n = N$ that for N prime, the mean for rank-1 lattice rules is (see also Theorem 3.3 with $n = N$)

$$\begin{aligned} \widehat{M}_{N,d} &= -\prod_{j=1}^{d}\beta_j + \frac{1}{N}\prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right) \\ &\quad + \frac{N-1}{N}\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-N^{1-\alpha})}{N-1}\right). \end{aligned}$$

Suppose we replace N by $N = \ell^r n$ in this last expression. This is not valid because N is not prime, but calculations using the correct (but more complicated) expression for the mean found in Theorem 5.3 indicate that this yields an underestimate of the true mean.

Now let

$$R_{n,d,\ell,r} := \frac{M_{n,d,copy(\ell,r)}}{\widehat{M}_{N,d}}.$$

As an indication of whether these intermediate-rank lattice rules are better than rank-1 lattice rules having approximately the same number of points, we would like a result which shows that $R_{n,d,\ell,r} < 1$. A preliminary result of this type is given in the following theorem.

Theorem 7.5 *Let n be a prime number such that $n \geq 1 + \frac{2\gamma_1}{\beta_1}\zeta(\alpha)$. If*

$$\rho_{\ell,r} := \prod_{j=1}^{r} \frac{\ell\beta_j + \frac{2\gamma_j\zeta(\alpha)}{\ell^{\alpha-1}}}{\beta_j + 2\gamma_j\zeta(\alpha)} < 1,$$

and

$$\begin{aligned}
&\ell^r(n-1)\prod_{j=1}^{r}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{(n-1)\ell^\alpha}\right)\prod_{j=r+1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right)\\
&< \ (\ell^r n-1)\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-(\ell^r n)^{1-\alpha})}{\ell^r n-1}\right), \qquad (7.2)
\end{aligned}$$

then

$$R_{n,d,\ell,r} < \rho_{\ell,r}.$$

Proof. By multiplying both $M_{n,d,copy(\ell,r)}$ and $\widehat{M}_{N,d}$ by $N = \ell^r n$, we can write

$$R_{n,d,\ell,r} = \frac{t_1 + t_2 - c}{b_1 + b_2 - c} \quad \text{and} \quad \rho_{\ell,r} = \frac{t_1}{b_1},$$

where

$$\begin{aligned}
t_1 &= \prod_{j=1}^{r}\left(\ell\beta_j + \frac{2\gamma_j\zeta(\alpha)}{\ell^{\alpha-1}}\right)\prod_{j=r+1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right),\\
t_2 &= \ell^r(n-1)\prod_{j=1}^{r}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{(n-1)\ell^\alpha}\right)\\
&\qquad \times \prod_{j=r+1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-n^{1-\alpha})}{n-1}\right),\\
b_1 &= \prod_{j=1}^{d}\left(\beta_j + 2\gamma_j\zeta(\alpha)\right),\\
b_2 &= (\ell^r n-1)\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)(1-(\ell^r n)^{1-\alpha})}{\ell^r n-1}\right),\\
c &= \ell^r n\prod_{j=1}^{d}\beta_j.
\end{aligned}$$

It is not hard to prove that

$$\frac{t_1 + t_2 - c}{b_1 + b_2 - c} < \frac{t_1}{b_1}$$

is true if b_1, b_2, t_1, t_2 and c are positive quantities satisfying

$$t_1 < b_1, \quad b_1 + b_2 > c, \quad \text{and} \quad t_2 < b_2 < c. \tag{7.3}$$

Thus the result is proved if we can prove that all these conditions hold.

It may not be obvious that b_2 and t_2 are positive quantities, but one can see that this is the case when $\beta_j - 2\gamma_j\zeta(\alpha)/(n-1) > 0$ for $j = 1, 2\ldots, d$ which is equivalent to the requirement on n given in the statement of the theorem. The requirement that $t_1 < b_1$ comes from the assumption that $\rho_{\ell,r} < 1$ while the requirement that $t_2 < b_2$ comes from the assumption given in (7.2). Also, it is clear that $b_2 < c$.

Let

$$\hat{b}_2 = (\ell^r n - 1)\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)}{\ell^r n - 1}\right).$$

It is clear that $b_2 > \hat{b}_2$. Thus we can prove that $b_1 + b_2 > c$ by proving that $b_1 + \hat{b}_2 - c > 0$. Using Lemma 3.5, we can write

$$\begin{aligned}
b_1 + \hat{b}_2 - c &= \prod_{j=1}^{d}(\beta_j + 2\gamma_j\zeta(\alpha)) + (\ell^r n - 1)\prod_{j=1}^{d}\left(\beta_j - \frac{2\gamma_j\zeta(\alpha)}{\ell^r n - 1}\right) - \ell^r n\prod_{j=1}^{d}\beta_j \\
&= \sum_{\emptyset\neq \mathrm{u}\subseteq\mathcal{D}}\left(\prod_{j\notin \mathrm{u}}\beta_j\prod_{j\in \mathrm{u}}(2\gamma_j\zeta(\alpha))\right) \\
&\quad +(\ell^r n - 1)\sum_{\emptyset\neq \mathrm{u}\subseteq\mathcal{D}}\left(\prod_{j\notin \mathrm{u}}\beta_j\prod_{j\in \mathrm{u}}\left(-\frac{2\gamma_j\zeta(\alpha)}{\ell^r n - 1}\right)\right) \\
&= \sum_{\emptyset\neq \mathrm{u}\subseteq\mathcal{D}}\left(V(\mathrm{u})\prod_{j\notin \mathrm{u}}\beta_j\prod_{j\in \mathrm{u}}(2\gamma_j\zeta(\alpha))\right),
\end{aligned}$$

where

$$V(\mathrm{u}) = 1 + (\ell^r n - 1)\left(-\frac{1}{\ell^r n - 1}\right)^{|\mathrm{u}|}$$

Clearly $V(\mathrm{u}) > 0$ if $|\mathrm{u}|$ is even. For $|\mathrm{u}| \geq 1$ odd, we have

$$V(\mathrm{u}) = 1 - (\ell^r n - 1)\left(\frac{1}{\ell^r n - 1}\right)^{|\mathrm{u}|} \geq 1 - 1 = 0.$$

Thus we conclude that $b_1 + \hat{b}_2 - c > 0$ and hence $b_1 + b_2 > c$. □

In the previous theorem, we made the assumption that $\rho_{\ell,r} < 1$ and that (7.2) was true. Attempts to prove that (7.2) is always true have not been successful. Our numerical test calculations with $\alpha = 2$, $\beta_j = 1$, and various choices of γ_j have indicated that (7.2) most likely does hold for $\ell = 2$ and small values of r. It may well be that (7.2) will not hold for large copy factors ℓ and large r. With this in mind, under the assumption that $\ell = 2$, the next result gives some sufficient conditions for $\rho_{2,r}$ to be less than one.

Lemma 7.6 *Let $\rho_{\ell,r}$ be defined as in Theorem 7.5 and set $\ell = 2$. If $\alpha \geq 2$ and*

$$\frac{\gamma_r}{\beta_r} > \frac{1}{(2 - 2^{2-\alpha})\zeta(\alpha)},$$

then $\rho_{2,r} < 1$.

Proof. A product of positive terms is guaranteed to be less than one when each of the terms is less than one. From the definition of $\rho_{\ell,r}$, we see that if $\ell = 2$, then this is the case when

$$\frac{2\beta_j + 2^{2-\alpha}\gamma_j\zeta(\alpha)}{\beta_j + 2\gamma_j\zeta(\alpha)} < 1.$$

When rearranged, this yields

$$\frac{\gamma_j}{\beta_j} > \frac{1}{(2 - 2^{2-\alpha})\zeta(\alpha)}.$$

Now since $\frac{\gamma_1}{\beta_1} \geq \frac{\gamma_2}{\beta_2} \geq \cdots$, the result follows. □

In the case when $\alpha = 2$, the condition of the lemma becomes

$$\frac{\gamma_r}{\beta_r} > \frac{1}{\zeta(2)} = \frac{6}{\pi^2} \approx 0.6079.$$

This suggests that when $\alpha = 2$, then it is worthwhile to take r to be at least one when $\frac{\gamma_1}{\beta_1} > \frac{6}{\pi^2}$.

7.1.4 Component-by-component construction

We now consider finding the components of the generating vector $\boldsymbol{z}$ one at a time. We shall see that with r fixed and weights properly chosen, such a construction results in intermediate-rank lattice rules which satisfy strong tractability error bounds.

Let $e_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$ denote the worst-case error for a QMC rule with the set of points

$$\left\{ \left(\boldsymbol{x}_i, \left\{ \frac{i z_{d+1}}{n} + \frac{m}{\ell} \right\} \right) : 0 \le i \le n-1,\, 0 \le m \le \ell - 1 \right\}.$$

Note that when $\ell = 1$, this set is just

$$\left\{ \left(\boldsymbol{x}_i, \left\{ \frac{i z_{d+1}}{n} \right\} \right) : 0 \le i \le n-1 \right\},$$

and in this case the theorem below is the same as Theorem 3.8.

Theorem 7.7 [cf. Theorem 3.8] *Let n be a prime number. Suppose there exist $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1} \in [0,1]^d$ such that*

$$e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \le \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + 4\gamma_j \zeta(\alpha) \right).$$

Then there exists $z_{d+1} \in \mathbb{Z}_n$ such that

$$e_{n,d+1,\ell}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \le \frac{1}{n} \prod_{j=1}^{d+1} \left(\beta_j + 4\gamma_j \zeta(\alpha) \right).$$

Such a z_{d+1} can be found by minimizing $e_{n,d+1,\ell}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$ over the set $\mathbb{Z}_n$.

Proof. Suppose that $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ satisfy the assumed bound. For any $z_{d+1} \in \mathbb{Z}_n$, it follows from Lemma 2.7 by a derivation similar to that used in the proof of Lemma 7.1 that

$$\begin{aligned}
&e_{n,d+1,\ell}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\
&= -\prod_{j=1}^{d+1} \beta_j + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h (x_{i,j} - x_{k,j})}}{|h|^\alpha} \right) \right. \\
&\qquad \left. \times \left(\beta_{d+1} + \frac{\gamma_{d+1}}{\ell^\alpha} \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h \ell (i-k) z_{d+1}/n}}{|h|^\alpha} \right) \right] \\
&= \beta_{d+1} e_{n,d}^2(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\
&\quad + \frac{\gamma_{d+1}}{\ell^\alpha n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h (x_{i,j} - x_{k,j})}}{|h|^\alpha} \right) \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h \ell (i-k) z_{d+1}/n}}{|h|^\alpha} \right].
\end{aligned}$$

Let us define the average

$$m_{n,d+1,\ell}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) := \frac{1}{n-1}\sum_{z_{d+1}\in\mathbb{Z}_n} e^2_{n,d+1,\ell}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1};z_{d+1}).$$

We see from the proof of Theorem 3.8 that the result is proved if we can prove that

$$m_{n,d+1,\ell}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \le \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j + 4\gamma_j\zeta(\alpha)\right).$$

It follows from the proof of Theorem 3.8 that

$$\begin{aligned} m_{n,d+1,\ell}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \;&\le\; \beta_{d+1}e^2_{n,d}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ &\quad + \frac{\gamma_{d+1}}{\ell^\alpha n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|T_\alpha(\ell(i-k),n)|\prod_{j=1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right). \end{aligned}$$

where $T_\alpha(k,n)$ is as given in Lemma 3.2. Now since $\ell \neq 0$ and $\gcd(\ell,n) = 1$, it follows from Lemma 3.2 and the proof of Theorem 3.8 that

$$\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}|T_\alpha(\ell(i-k),n)| = \sum_{i=0}^{n-1}|T_\alpha(0,n)| + \sum_{i=0}^{n-1}\sum_{\substack{k=0\\k\neq i}}^{n-1}|T_\alpha(\ell(i-k),n)| \le 4\zeta(\alpha)n.$$

Hence

$$\begin{aligned} &m_{n,d+1,\ell}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_{n-1}) \\ &\le\; \beta_{d+1}\times\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+4\gamma_j\zeta(\alpha)\right) + \frac{4\gamma_{d+1}\zeta(\alpha)}{\ell^\alpha n}\prod_{j=1}^{d}\left(\beta_j+2\gamma_j\zeta(\alpha)\right) \\ &\le\; \frac{1}{n}\prod_{j=1}^{d+1}\left(\beta_j+4\gamma_j\zeta(\alpha)\right). \end{aligned}$$

This completes the proof. □

Corollary 7.8 *Let n be a prime number and let $1 \le r \le d$. We can construct $\boldsymbol{z} \in \mathbb{Z}_n^d$ component-by-component such that for all $s = 1,\ldots,d$,*

$$e^2_{n,s,copy(\ell,\min(r,s))}(z_1,\ldots,z_s) \le \frac{1}{n}\prod_{j=1}^{s}\left(\beta_j+4\gamma_j\zeta(\alpha)\right).$$

We can set $z_1 = 1$, and for s satisfying $1 \le s \le d$, each z_s can be found by minimizing $e^2_{n,s,copy(\ell,\min(r,s))}(z_1,\ldots,z_s)$ over the set $\mathbb{Z}_n$.

Proof. In one dimension, we may take $z_1 = 1$ and obtain

$$e^2_{n,1,copy(\ell,1)}(z_1) = e^2_{n,1,copy(\ell,1)}(1) = \frac{2\gamma_1\zeta(\alpha)}{\ell^\alpha n^\alpha} \le \frac{1}{n}\left(\beta_1 + 4\gamma_1\zeta(\alpha)\right).$$

For each $s = 2, \ldots, r$, it follows from Theorem 7.7 inductively with $d = s-1$ that z_s can be found by minimizing $e^2_{n,s,copy(\ell,s)}(z_1, \ldots, z_s)$ over the set $\mathbb{Z}_n$ and that this choice satisfies the desired bound. Now for each $s = r+1, \ldots, d$, it follows again from Theorem 7.7 inductively with $d = s-1$ and $\ell = 1$, that z_s can be found by minimizing $e^2_{n,s,copy(\ell,r)}(z_1, \ldots, z_s)$ over the set $\mathbb{Z}_n$ and as before, this choice of z_s satisfies the desired bound. □

Given a fixed r, the above corollary leads us to the following algorithm for constructing intermediate-rank lattice rules with square worst-case error bounded by an expression of the form given in Theorem 2.9 with $a = 4\zeta(\alpha)$ and $b = \ell^r$ (recall that the total number of quadrature points is $N = \ell^r n$).

Algorithm 7.9 *Given n a prime number and $1 \le r \le d$:*

1. *Set z_1, the first component of $\boldsymbol{z}$, to 1.*

2. *For $s = 2, 3, \ldots, r-1, r$, find $z_s \in \mathbb{Z}_n = \{1, 2, \ldots, n-1\}$ such that*

$$e^2_{n,s,copy(\ell,s)}(z_1, \ldots, z_s) = -\prod_{j=1}^{s}\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left(\beta_j + \frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h\ell k z_j/n}}{|h|^\alpha}\right)$$

is minimized.

3. *For $s = r+1, r+2, \ldots, d-1, d$, find $z_s \in \mathbb{Z}_n = \{1, 2, \ldots, n-1\}$ such that*

$$\begin{aligned} & e^2_{n,s,copy(\ell,r)}(z_1, \ldots, z_s) \\ = & -\prod_{j=1}^{s}\beta_j + \frac{1}{n}\sum_{k=0}^{n-1}\left[\prod_{j=1}^{r}\left(\beta_j + \frac{\gamma_j}{\ell^\alpha}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h\ell k z_j/n}}{|h|^\alpha}\right)\right. \\ & \qquad \left. \times \prod_{j=r+1}^{s}\left(\beta_j + \gamma_j\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z_j/n}}{|h|^\alpha}\right)\right] \end{aligned}$$

is minimized.

7.2 Shifted intermediate-rank lattice rules in weighted Sobolev spaces

Now we change the function spaces to weighted Sobolev spaces. We consider the $\boldsymbol{\Delta}$-shift of the (ℓ, r)-copy of a rank-1 lattice rule with generating vector $\boldsymbol{z}$, that is, a rule with points given by

$$\left\{ \left\{ \frac{i\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell} + \boldsymbol{\Delta} \right\} : 0 \leq i \leq n-1, \right.$$
$$\left. 0 \leq m_1, \ldots, m_r \leq \ell - 1 \right\},$$

where $\ell \geq 1$, $\gcd(\ell, n) = 1$, and $0 \leq r \leq d$. Let $e_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta})$ denote the worst-case error for such a rule. An expression for $e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta})$ can be derived from Lemma 2.16.

Here we give just the general ideas of the existence and the construction of a good shifted intermediate-rank lattice rule. The full details follow closely the arguments from Chapter 4.

To obtain an upper bound on the square worst-case error, we define the mean of $e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta})$ over all values of $\boldsymbol{z} \in \mathbb{Z}_n^d$ and $\boldsymbol{\Delta} \in [0,1]^d$ by

$$M_{n,d,copy(\ell,r)} := \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathbb{Z}_n^d} \left(\int_{[0,1]^d} e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta}) \, \mathrm{d}\boldsymbol{\Delta} \right).$$

Using the known relationship between weighted Korobov spaces and weighted Sobolev spaces (see Lemmas 2.4 and 2.12), we see that this mean is exactly the mean given in Theorem 7.2 with α replaced by 2, β_j replaced by $\beta_j + \frac{\gamma_j}{3}$ and γ_j replaced by $\frac{\gamma_j}{2\pi^2}$. An upper bound for $M_{n,d,copy(\ell,r)}$ follows in the same way from Theorem 7.3:

$$\frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{2} \right).$$

From this we conclude that there exists at least one pair $(\boldsymbol{z}, \boldsymbol{\Delta})$ such that $e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta})$ is bounded by this upper bound on the mean. Since this bound is of the form given in Theorem 2.15, we conclude that *the family of shifted intermediate-rank lattice rules (with n prime) is strongly tractable in* *weighted Sobolev spaces if and only if*

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty.$$

Let $e_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$ denote the worst-case error for a QMC rule with the set of points

$$\left\{ \left(\boldsymbol{x}_i, \left\{ \frac{i z_{d+1}}{n} + \frac{m}{\ell} + \Delta_{d+1} \right\} \right) : 0 \le i \le n-1,\, 0 \le m \le \ell - 1 \right\}.$$

To construct the pair (z_{d+1}, Δ_{d+1}) component-by-component, we define the following means:

$$\begin{aligned} \omega_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) &:= \int_0^1 e^2_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})\, \mathrm{d}\Delta_{d+1}, \\ \widetilde{\omega}_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) &:= \frac{1}{n} \sum_{m=1}^{n} e^2_{n,d+1,\ell} \left(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \tfrac{2m-1}{2n} \right), \\ m_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) &:= \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} \omega_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}). \end{aligned}$$

With some involved algebraic manipulations, we can show that for $\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}$ satisfying

$$e^2_{n,d}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \le \frac{1}{n} \prod_{j=1}^{d} (\beta_j + \gamma_j),$$

we can choose $z_{d+1} \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ to minimize $\omega_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1})$, and then (with this z_{d+1} fixed) choose $\Delta_{d+1} \in \left\{ \frac{2m-1}{2n} : 1 \le m \le n-1 \right\}$ to minimize $e^2_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1})$. Such choices will satisfy

$$\begin{aligned} e^2_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}, \Delta_{d+1}) &\le \widetilde{\omega}_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\ &\le \omega_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}; z_{d+1}) \\ &\le m_{n,d+1,\ell}(\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{n-1}) \\ &\le \frac{1}{n} \prod_{j=1}^{d+1} (\beta_j + \gamma_j). \end{aligned}$$

Note that the result also holds for $\ell = 1$, that is, no 'copying' in the $(d+1)$-th dimension. For $d = 1$, we can show that there exists (z_1, Δ_1) satisfying

$$e^2_{n,1,copy(\ell,1)}(z_1, \Delta_1) \le \frac{1}{n} (\beta_1 + \gamma_1).$$

All of the above lead us to the following algorithm for constructing a pair $(\boldsymbol{z}, \boldsymbol{\Delta})$ such that for all $s = 1, \ldots, d$,

$$e^2_{n,s,copy(\ell,\min(r,s))}\left((z_1, \ldots, z_s), (\Delta_1, \ldots, \Delta_s)\right) \leq \frac{1}{n}\prod_{j=1}^{s}(\beta_j + \gamma_j)\,.$$

Algorithm 7.10 *Given n a prime number and $1 \leq r \leq d$:*

1. *Set z_1, the first component of $\boldsymbol{z}$, to 1.*

2. *Find $\Delta_1 \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize $e^2_{n,1,copy(\ell,1)}(z_1, \Delta_1)$.*

3. *For $s = 2, 3, \ldots, r-1, r$, do the following:*

   (a) *Find $z_s \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ to minimize*

   $$\omega_{n,s,copy(\ell,s)}\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1}); z_s\right).$$

   (b) *Find $\Delta_s \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize*

   $$e^2_{n,s,copy(\ell,s)}\left((z_1, \ldots, z_s), (\Delta_1, \ldots, \Delta_s)\right).$$

4. *For $s = r+1, r+2, \ldots, d-1, d$, do the following:*

   (a) *Find $z_s \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ to minimize*

   $$\omega_{n,s,copy(\ell,r)}\left((z_1, \ldots, z_{s-1}), (\Delta_1, \ldots, \Delta_{s-1}); z_s\right).$$

   (b) *Find $\Delta_s \in \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}$ to minimize*

   $$e^2_{n,s,copy(\ell,r)}\left((z_1, \ldots, z_s), (\Delta_1, \ldots, \Delta_s)\right).$$

The cost for the construction is $O(n^3d^2)$ operations and it is dominated by the construction of the shift. In Chapter 6 the idea of using a number of random shifts was introduced. This not only cuts the cost of the construction down to $O(n^2d^2)$ operations, it also allows error estimation. Following Chapter 6, we can construct the generating vector component-by-component by minimizing over the quantity

$$\hat{e}^2_{n,d,copy(\ell,r)}(\boldsymbol{z}) := \int_{[0,1]^d} e^2_{n,d,copy(\ell,r)}(\boldsymbol{z}, \boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta}.$$

We give the algorithm below.

Algorithm 7.11 *Given n a prime number and $1 \le r \le d$:*

1. *Set z_1, the first component of $\boldsymbol{z}$, to 1.*

2. *For $s = 2, 3, \ldots, r-1, r$, find $z_s \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ to minimize*

$$\hat{e}^2_{n,d,copy(\ell,s)}(z_1, \ldots, z_s).$$

3. *For $s = r+1, r+2, \ldots, d-1, d$, find $z_s \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ to minimize*

$$\hat{e}^2_{n,d,copy(\ell,r)}(z_1, \ldots, z_s).$$

Chapter 8

Constructing Randomly Shifted Rank-1 Lattice Rules in Weighted Sobolev Spaces When $n = pq$

In Algorithm 6.4, the cost for constructing an n-point randomly shifted rank-1 lattice rule in up to d dimensions is $O(n^2d^2)$ operations, where n is a prime number. Here we consider the situation when n is the product of two distinct prime numbers p and q. We still generate the shifts randomly but now the cost of constructing the two generating vectors component-by-component is only $O(n(p+q)d^2)$ operations, and in the case of p and q being roughly the same, it is $O(n^{1.5}d^2)$ operations. When the sum of γ_j/β_j is finite, the rules constructed again achieve a worst-case strong tractability error bound in a probabilistic sense (see Chapter 6).

8.1 The existence of good rules

Instead of taking n to be a prime number, we choose n to be the product of two distinct prime numbers p and q. We are thus considering rank-1 lattice rules with points given by the set

$$\left\{\left\{\frac{iz}{p}+\frac{kw}{q}\right\} : 0 \le i \le p-1,\, 0 \le k \le q-1\right\},$$

where $\boldsymbol{z} \in \mathbb{Z}_p^d = \{1,2,\ldots,p-1\}^d$ and $\boldsymbol{w} \in \mathbb{Z}_q^d = \{1,2,\ldots,q-1\}^d$ are two generating vectors. The idea of using the decomposition $n = pq$ is not new. In 1960, Korobov pointed out in [18] that by taking q to be roughly $\sqrt{p}$, the cost of calculating a quantity similar to our square worst-case error is reduced from $O(n^2 d)$ operations to $O(n^{\frac{4}{3}} d)$ operations. This fact was later mentioned again in Hua and Wang's book [13].

It follows from a generalization of (6.2) that the worst-case error satisfies

$$\begin{aligned}
&\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w})\\
&= -\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right)+\frac{1}{pq}\sum_{i=0}^{p-1}\sum_{k=0}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}+\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&= -\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right)+\frac{1}{pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)\\
&\quad+\frac{1}{pq}\sum_{i=1}^{p-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad+\frac{1}{pq}\sum_{k=1}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad+\frac{1}{pq}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}+\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right). \qquad (8.1)
\end{aligned}$$

8.1.1 Means when $n = pq$

We define the following means of the square worst-case error:

$$\begin{aligned}
\hat{\Omega}_{p,q,d}(\boldsymbol{w}) &:= \frac{1}{(p-1)^d}\sum_{\boldsymbol{z}\in\mathbb{Z}_p^d}\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}),\\
\hat{\Theta}_{p,q,d}(\boldsymbol{z}) &:= \frac{1}{(q-1)^d}\sum_{\boldsymbol{w}\in\mathbb{Z}_q^d}\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}),\\
\hat{M}_{p,q,d} &:= \frac{1}{(p-1)^d(q-1)^d}\sum_{\boldsymbol{z}\in\mathbb{Z}_p^d}\sum_{\boldsymbol{w}\in\mathbb{Z}_q^d}\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}).
\end{aligned}$$

To derive the explicit expressions for these means, we need to make use of the following result:

Lemma 8.1 *For $1 \le i \le p-1$ and $1 \le k \le q-1$, we have*

$$\frac{1}{p-1}\sum_{z=1}^{p-1} B_2\left(\left\{\tfrac{iz}{p}\right\}\right) = -\frac{1}{6p},$$

$$\frac{1}{p-1}\sum_{z=1}^{p-1} B_2\left(\left\{\tfrac{iz}{p}+\tfrac{kw}{q}\right\}\right) = \frac{1}{p(p-1)}B_2\left(\left\{\tfrac{pkw}{q}\right\}\right) - \frac{1}{p-1}B_2\left(\left\{\tfrac{kw}{q}\right\}\right),$$

and

$$\frac{1}{(p-1)(q-1)}\sum_{z=1}^{p-1}\sum_{w=1}^{q-1} B_2\left(\left\{\tfrac{iz}{p}+\tfrac{kw}{q}\right\}\right) = \frac{1}{6pq}.$$

Proof. For $1 \le i \le p-1$, the result

$$\frac{1}{p-1}\sum_{z=1}^{p-1} B_2\left(\left\{\tfrac{iz}{p}\right\}\right) = -\frac{1}{6p}$$

was already obtained in (6.3).

Using (2.8) with $\alpha = 2$, and the property that

$$\frac{1}{p-1}\sum_{z=1}^{p-1} e^{2\pi i h z/p} = \begin{cases} 1, & \text{if } h \text{ is a multiple of } p, \\ -\frac{1}{p-1}, & \text{otherwise,} \end{cases}$$

we can write, for $1 \le i \le p-1$ and $1 \le k \le q-1$,

$$\begin{aligned}
&\frac{1}{p-1}\sum_{z=1}^{p-1} B_2\left(\left\{\tfrac{iz}{p}+\tfrac{kw}{q}\right\}\right) \\
&= \frac{1}{p-1}\sum_{z=1}^{p-1}\left(\frac{1}{2\pi^2}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h(iz/p+kw/q)}}{h^2}\right) \\
&= \frac{1}{2\pi^2}\sum_{h=-\infty}^{\infty}{}' \left[\frac{e^{2\pi i h k w/q}}{h^2}\left(\frac{1}{p-1}\sum_{z=1}^{p-1} e^{2\pi i h i z/p}\right)\right] \\
&= \frac{1}{2\pi^2}\left[\sum_{h\equiv 0\ (\text{ mod } p)}{}' \frac{e^{2\pi i h k w/q}}{h^2} - \frac{1}{p-1}\sum_{h\not\equiv 0\ (\text{ mod } p)}{}' \frac{e^{2\pi i h k w/q}}{h^2}\right] \\
&= \frac{1}{2\pi^2}\left[\sum_{m=-\infty}^{\infty}{}' \frac{e^{2\pi i m p k w/q}}{m^2p^2} - \frac{1}{p-1}\left(\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k w/q}}{h^2} - \sum_{m=-\infty}^{\infty}{}' \frac{e^{2\pi i m p k w/q}}{m^2p^2}\right)\right] \\
&= \frac{1}{2\pi^2}\left[\frac{1}{p^2}\left(1+\frac{1}{p-1}\right)\sum_{m=-\infty}^{\infty}{}' \frac{e^{2\pi i m p k w/q}}{m^2} - \frac{1}{p-1}\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k w/q}}{h^2}\right] \\
&= \frac{1}{p(p-1)}B_2\left(\left\{\tfrac{pkw}{q}\right\}\right) - \frac{1}{p-1}B_2\left(\left\{\tfrac{kw}{q}\right\}\right).
\end{aligned}$$

Finally, for $1 \leq i \leq p-1$ and $1 \leq k \leq q-1$,

$$\begin{aligned}
&\frac{1}{(p-1)(q-1)} \sum_{z=1}^{p-1} \sum_{w=1}^{q-1} B_2\left(\left\{\tfrac{iz}{p} + \tfrac{kw}{q}\right\}\right) \\
&= \frac{1}{q-1} \sum_{w=1}^{q-1} \left[\frac{1}{p(p-1)} B_2\left(\left\{\tfrac{pkw}{q}\right\}\right) - \frac{1}{p-1} B_2\left(\left\{\tfrac{kw}{q}\right\}\right)\right] \\
&= \frac{1}{p(p-1)}\left(-\frac{1}{6q}\right) - \frac{1}{p-1}\left(-\frac{1}{6q}\right) = \frac{1}{6pq}.
\end{aligned}$$

This completes the proof. □

Here we give the explicit expressions for the various means defined earlier.

Theorem 8.2 *Let p and q be distinct prime numbers. We have*

$$\begin{aligned}
&\hat{\Omega}_{p,q,d}(\boldsymbol{w}) \\
&= -\prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{3}\right) + \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) + \frac{p-1}{pq} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6p}\right)\right) \\
&+ \frac{1}{pq} \sum_{k=1}^{q-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right) \\
&+ \frac{p-1}{pq} \sum_{k=1}^{q-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left[\tfrac{1}{p(p-1)} B_2\left(\left\{\tfrac{pkw_j}{q}\right\}\right) - \frac{1}{p-1} B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right),
\end{aligned}$$

$$\begin{aligned}
&\hat{\Theta}_{p,q,d}(\boldsymbol{z}) \\
&= -\prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{3}\right) + \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) + \frac{q-1}{pq} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6q}\right)\right) \\
&+ \frac{1}{pq} \sum_{i=1}^{p-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right) \\
&+ \frac{q-1}{pq} \sum_{i=1}^{p-1} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left[\tfrac{1}{q(q-1)} B_2\left(\left\{\tfrac{qiz_j}{p}\right\}\right) - \frac{1}{q-1} B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right),
\end{aligned}$$

and

$$\begin{aligned}
&\hat{M}_{p,q,d} \\
&= -\prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{3}\right) + \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) + \frac{p-1}{pq} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6p}\right)\right) \\
&+ \frac{q-1}{pq} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6q}\right)\right) + \frac{(p-1)(q-1)}{pq} \prod_{j=1}^{d} \left(\beta_j + \gamma_j\left(\tfrac{1}{3} + \tfrac{1}{6pq}\right)\right),
\end{aligned}$$

Proof. From (8.1) we can derive the expressions for $\hat{\Omega}_{p,q,d}(\boldsymbol{w})$ and $\hat{\Theta}_{p,q,d}(\boldsymbol{z})$ using Lemma 8.1. The expression for $\hat{M}_{p,q,d}$ can then be derived using either

$$\hat{M}_{p,q,d} = \frac{1}{(q-1)^d}\sum_{\boldsymbol{w}\in\mathbb{Z}_q^d}\hat{\Omega}_{p,q,d}(\boldsymbol{w}) \quad \text{or} \quad \hat{M}_{p,q,d} = \frac{1}{(p-1)^d}\sum_{\boldsymbol{z}\in\mathbb{Z}_p^d}\hat{\Theta}_{p,q,d}(\boldsymbol{z}),$$

and applying Lemma 8.1 again. □

8.1.2 Upper bound when $n = pq$

Now we find an upper bound for the mean $\hat{M}_{p,q,d}$.

Theorem 8.3 *Let p and q be distinct prime numbers. We have*

$$\begin{aligned}\hat{M}_{p,q,d} &\le \frac{2}{pq}\left(\prod_{j=1}^{d}(\beta_j + \tfrac{\gamma_j}{2}) - \prod_{j=1}^{d}(\beta_j + \tfrac{\gamma_j}{3})\right)\\ &\le \min\left(\frac{2}{pq}\prod_{j=1}^{d}(\beta_j + \tfrac{\gamma_j}{2}), \frac{1}{pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{2\gamma_j}{3}\right)\right).\end{aligned}$$

Proof. Using Lemma 3.5, we can write $\hat{M}_{p,q,d}$ from Theorem 8.2 as

$$\begin{aligned}\hat{M}_{p,q,d} &= \frac{1}{pq}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}(\beta_j + \tfrac{\gamma_j}{3})\prod_{j\in\mathfrak{u}}(\tfrac{\gamma_j}{6})\right]\\ &\quad+\frac{p-1}{pq}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}(\beta_j + \tfrac{\gamma_j}{3})\prod_{j\in\mathfrak{u}}\left(-\tfrac{\gamma_j}{6p}\right)\right]\\ &\quad+\frac{q-1}{pq}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}(\beta_j + \tfrac{\gamma_j}{3})\prod_{j\in\mathfrak{u}}\left(-\tfrac{\gamma_j}{6q}\right)\right]\\ &\quad+\frac{(p-1)(q-1)}{pq}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left[\prod_{j\notin\mathfrak{u}}(\beta_j + \tfrac{\gamma_j}{3})\prod_{j\in\mathfrak{u}}\left(\tfrac{\gamma_j}{6pq}\right)\right]\\ &= \frac{1}{pq}\sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}}\left[U(\mathfrak{u})\prod_{j\notin\mathfrak{u}}(\beta_j + \tfrac{\gamma_j}{3})\prod_{j\in\mathfrak{u}}(\tfrac{\gamma_j}{6})\right],\end{aligned}$$

where

$$U(\mathfrak{u}) = 1 + (p-1)\left(-\tfrac{1}{p}\right)^{|\mathfrak{u}|} + (q-1)\left(-\tfrac{1}{q}\right)^{|\mathfrak{u}|} + (p-1)(q-1)\left(\tfrac{1}{pq}\right)^{|\mathfrak{u}|}.$$

For $1 \le |\mathfrak{u}| \le d$, if $|\mathfrak{u}|$ is even we have

$$U(\mathfrak{u}) \le 1 + \frac{p-1}{p^2} + \frac{q-1}{q^2} + \frac{(p-1)(q-1)}{p^2q^2} \le 1 + \frac{1}{p} + \frac{1}{q} + \frac{1}{pq} \le 2,$$

and if $|\mathrm{u}|$ is odd we have

$$U(\mathrm{u}) \leq 1 + \frac{(p-1)(q-1)}{pq} \leq 2.$$

Thus we have $U(\mathrm{u}) \leq 2$ for all u and so

$$\begin{aligned} \hat{M}_{p,q,d} &\leq \frac{2}{pq} \sum_{\emptyset \neq \mathrm{u} \subseteq \mathcal{D}} \left(\prod_{j \notin \mathrm{u}} (\beta_j + \tfrac{\gamma_j}{3}) \prod_{j \in \mathrm{u}} (\tfrac{\gamma_j}{6}) \right) \\ &= \frac{2}{pq} \left(\prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{2}) - \prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{3}) \right) \leq \frac{2}{pq} \prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{2}) . \end{aligned}$$

Also, we have

$$\begin{aligned} \frac{2}{pq} \sum_{\emptyset \neq \mathrm{u} \subseteq \mathcal{D}} \left(\prod_{j \notin \mathrm{u}} (\beta_j + \tfrac{\gamma_j}{3}) \prod_{j \in \mathrm{u}} (\tfrac{\gamma_j}{6}) \right) &\leq \frac{1}{pq} \sum_{\emptyset \neq \mathrm{u} \subseteq \mathcal{D}} \left(\prod_{j \notin \mathrm{u}} (\beta_j + \tfrac{\gamma_j}{3}) \prod_{j \in \mathrm{u}} (\tfrac{\gamma_j}{3}) \right) \\ &= \frac{1}{pq} \left(\prod_{j=1}^{d} \left(\beta_j + \tfrac{2\gamma_j}{3}\right) - \prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{3}) \right) \\ &\leq \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{2\gamma_j}{3}\right) . \end{aligned}$$

This completes the proof. □

Corollary 8.4 *Let p and q be distinct prime numbers. Then there exist a choice of $\boldsymbol{z} \in \mathbb{Z}_p^d$ and a choice of $\boldsymbol{w} \in \mathbb{Z}_q^d$ such that*

$$\begin{aligned} \hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) &\leq \frac{2}{pq} \left(\prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{3}) - \prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{3}) \right) \\ &\leq \min \left(\frac{2}{pq} \prod_{j=1}^{d} (\beta_j + \tfrac{\gamma_j}{3}) , \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{2\gamma_j}{3}\right) \right) . \end{aligned}$$

Proof. Since $\hat{M}_{p,q,d}$ is the average of $\hat{\Theta}_{p,q,d}(\boldsymbol{z})$ over all $\boldsymbol{z} \in \mathbb{Z}_p^d$, there exists a $\boldsymbol{z}$ such that

$$\hat{\Theta}_{p,q,d}(\boldsymbol{z}) \leq \hat{M}_{p,q,d}.$$

Now for this $\boldsymbol{z}$, since $\hat{\Theta}_{p,q,d}(\boldsymbol{z})$ is the average of $\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w})$ over all $\boldsymbol{w} \in \mathbb{Z}_q^d$, there exists a $\boldsymbol{w}$ such that

$$\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) \leq \hat{\Theta}_{p,q,d}(\boldsymbol{z}),$$

and in turn, by Theorem 8.3, this pair of $(\boldsymbol{z}, \boldsymbol{w})$ will satisfy

$$\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) \leq \hat{M}_{p,q,d} \leq \min\left(\frac{2}{pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right), \frac{1}{pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{2\gamma_j}{3}\right)\right).$$

This completes the proof. □

We remark that both expressions in the minimum function are of the form given in Theorem 2.15.

8.2 Component-by-component construction

In this section we propose two algorithms for constructing randomly shifted rank-1 lattice rules when $n = pq$: the 'partial search' and the 'separate search'. The partial search algorithm is theoretically justified while the separate search algorithm is not.

8.2.1 The theoretical foundation and the algorithm

Here we give the theoretical foundation for the construction of a randomly shifted rank-1 lattice rule that satisfies the bound

$$\frac{1}{pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{2\gamma_j}{3}\right).$$

We define the following means over the $(d+1)$-th component of the generating vectors

$$\begin{aligned}
\hat{\rho}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; w_{d+1}) &:= \frac{1}{p-1}\sum_{z_{d+1}=1}^{p-1} \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right), \\
\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1}) &:= \frac{1}{q-1}\sum_{w_{d+1}=1}^{q-1} \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right),
\end{aligned}$$

and

$$\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}) := \frac{1}{(p-1)(q-1)}\sum_{z_{d+1}=1}^{p-1}\sum_{w_{d+1}=1}^{q-1} \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right).$$

Theorem 8.5 *Let p and q be distinct prime numbers. We have*

$$\begin{aligned}
&\hat{\rho}_{p,q,d+1}(\boldsymbol{z},\boldsymbol{w};w_{d+1})\\
&= \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w})+\frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)\\
&\quad -\frac{\gamma_{d+1}}{6p^2q}\sum_{i=1}^{p-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad +\frac{\gamma_{d+1}}{pq}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)B_2\left(\left\{\tfrac{kw_{d+1}}{q}\right\}\right)\right]\\
&\quad +\frac{\gamma_{d+1}}{pq}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}+\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\right.\\
&\qquad\qquad \left.\times\left(\tfrac{1}{p(p-1)}B_2\left(\left\{\tfrac{pkw_{d+1}}{q}\right\}\right)-\tfrac{1}{p-1}B_2\left(\left\{\tfrac{kw_{d+1}}{q}\right\}\right)\right)\right],
\end{aligned}$$

$$\begin{aligned}
&\hat{\theta}_{p,q,d+1}(\boldsymbol{z},\boldsymbol{w};z_{d+1})\\
&= \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w})+\frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)\\
&\quad +\frac{\gamma_{d+1}}{pq}\sum_{i=1}^{p-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right)+\tfrac{1}{3}\right]\right)B_2\left(\left\{\tfrac{iz_{d+1}}{p}\right\}\right)\right]\\
&\quad -\frac{\gamma_{d+1}}{6pq^2}\sum_{k=1}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad +\frac{\gamma_{d+1}}{pq}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}+\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\right.\\
&\qquad\qquad \left.\times\left(\tfrac{1}{q(q-1)}B_2\left(\left\{\tfrac{qiz_{d+1}}{p}\right\}\right)-\tfrac{1}{q-1}B_2\left(\left\{\tfrac{iz_{d+1}}{p}\right\}\right)\right)\right],
\end{aligned}$$

and

$$\begin{aligned}
\hat{m}_{p,q,d+1}(\boldsymbol{z},\boldsymbol{w}) &= \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w})+\frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)\\
&\quad -\frac{\gamma_{d+1}}{6p^2q}\sum_{i=1}^{p-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad -\frac{\gamma_{d+1}}{6pq^2}\sum_{k=1}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right)\\
&\quad +\frac{\gamma_{d+1}}{6p^2q^2}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}+\tfrac{kw_j}{q}\right\}\right)+\tfrac{1}{3}\right]\right).
\end{aligned}$$

Proof. Using (8.1), we can write

$$
\begin{aligned}
&\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \\
&= \left(\beta_{d+1} + \frac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) + \frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{2}\right) \\
&+ \frac{\gamma_{d+1}}{pq}\sum_{i=1}^{p-1}\left[\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right)B_2\left(\left\{\tfrac{iz_{d+1}}{p}\right\}\right)\right] \\
&+ \frac{\gamma_{d+1}}{pq}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right)B_2\left(\left\{\tfrac{kw_{d+1}}{q}\right\}\right)\right] \\
&+ \frac{\gamma_{d+1}}{pq}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right)\right. \\
&\qquad\qquad \left.\times B_2\left(\left\{\tfrac{iz_{d+1}}{p} + \tfrac{kw_{d+1}}{q}\right\}\right)\right].
\end{aligned}
$$

From this we can derive the expressions for the means $\hat{\rho}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; w_{d+1})$ and $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ using Lemma 8.1. The expression for $\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w})$ can then be derived using either

$$\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}) = \frac{1}{q-1}\sum_{w_{d+1}=1}^{q-1}\hat{\rho}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; w_{d+1}),$$

or

$$\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}) = \frac{1}{p-1}\sum_{z_{d+1}=1}^{p-1}\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1}),$$

and applying Lemma 8.1 again. □

The following theorem gives the theoretical foundation for the component-by-component search.

Theorem 8.6 *Let p and q be two distinct prime numbers. Suppose there exist $\boldsymbol{z} \in \mathbb{Z}_p^d$ and $\boldsymbol{w} \in \mathbb{Z}_q^d$ such that*

$$\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) \leq \frac{1}{pq}\prod_{j=1}^{d}\left(\beta_j + \tfrac{2\gamma_j}{3}\right).$$

Then there exist $z_{d+1} \in \mathbb{Z}_p$ and $w_{d+1} \in \mathbb{Z}_q$ such that

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \leq \frac{1}{pq}\prod_{j=1}^{d+1}\left(\beta_j + \tfrac{2\gamma_j}{3}\right).$$

A pair (z_{d+1}, w_{d+1}) satisfying this bound can be found by first minimizing $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ over all $z_{d+1} \in \mathbb{Z}_p$ and then (with this z_{d+1} fixed) minimizing $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$ over all $w_{d+1} \in \mathbb{Z}_q$. Moreover, the bound holds for $d = 1$.

Proof. Suppose that the pair $(\boldsymbol{z}, \boldsymbol{w})$ satisfies the assumed bound. Since

$$\tfrac{1}{4} \leq B_2(x) + \tfrac{1}{3} \leq \tfrac{1}{2},$$

we have from Theorem 8.5 that

$$\begin{aligned}
&\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}) \\
&\leq \left(\beta_{d+1} + \tfrac{\gamma_{d+1}}{3}\right) \hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) + \frac{\gamma_{d+1}}{3pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) \\
&\leq \left(\beta_{d+1} + \tfrac{\gamma_{d+1}}{3}\right) \times \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{2\gamma_j}{3}\right) + \frac{\gamma_{d+1}}{3} \times \frac{1}{pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) \\
&\leq \frac{1}{pq} \prod_{j=1}^{d+1} \left(\beta_j + \tfrac{2\gamma_j}{3}\right).
\end{aligned}$$

Now since $\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w})$ is the average of $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ over all $z_{d+1} \in \mathbb{Z}_p$, we can choose $z_{d+1} \in \mathbb{Z}_p$ to minimize $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ and this z_{d+1} will satisfy

$$\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1}) \leq \hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}).$$

With this z_{d+1} fixed, since $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ is the average over all $w_{d+1} \in \mathbb{Z}_q$ of $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$, we can choose $w_{d+1} \in \mathbb{Z}_q$ to minimize $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$ and this w_{d+1} will satisfy

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \leq \hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1}),$$

and in turn we have

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \leq \frac{1}{pq} \prod_{j=1}^{d+1} \left(\beta_j + \tfrac{2\gamma_j}{3}\right).$$

In one dimension, there is only one n-point lattice rule, namely, the n-point rectangle rule. Thus we may take $z_1 = 1$ and $w_1 = 1$ to obtain

$$\begin{aligned}
\hat{e}^2_{p,q,1}(1,1) &= \hat{M}_{p,q,1} \\
&= -\left(\beta_1 + \tfrac{\gamma_1}{3}\right) + \tfrac{1}{pq}\left(\beta_1 + \tfrac{\gamma_1}{2}\right) + \tfrac{p-1}{pq}\left(\beta_1 + \gamma_1\left(\tfrac{1}{3} - \tfrac{1}{6p}\right)\right) \\
&\quad + \tfrac{q-1}{pq}\left(\beta_1 + \gamma_1\left(\tfrac{1}{3} - \tfrac{1}{6q}\right)\right) + \tfrac{(p-1)(q-1)}{pq}\left(\beta_1 + \gamma_1\left(\tfrac{1}{3} + \tfrac{1}{6pq}\right)\right) \\
&= \frac{\gamma_1}{6p^2q^2} \le \frac{1}{pq}\left(\beta_1 + \tfrac{2\gamma_1}{3}\right).
\end{aligned}$$

Hence the bound holds for $d = 1$. □

For the $(d+1)$-th dimension, according to the previous theorem, we first search for z_{d+1} to minimize $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ and the cost is $O(p^2qd)$ operations. We then search for w_{d+1} to minimize $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$ and the cost is $O(pq^2d)$ operations. Thus it requires $O(n(p+q)d)$ operations to construct each pair (z_{d+1}, w_{d+1}). Alternatively, we could search for w_{d+1} to minimize $\hat{\rho}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; w_{d+1})$ first and then search for z_{d+1} to minimize $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$. In both cases, the cost for constructing a n-point rule up to dimension d is $O(n(p+q)d^2)$ operations. Similar to other component-by-component algorithms, this cost can be reduced to $O(n(p+q)d)$ operations at the expense of $O(n)$ storage.

Using the symmetric property of B_2, we have

$$\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1}) = \hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; p - z_{d+1}).$$

Thus the search of z_{d+1} can be reduced to the set $\left\{1, 2, \ldots, \frac{p-1}{2}\right\}$.

Algorithm 8.7 [Partial Search]

Given two distinct prime numbers p and q:

1. *Set z_1 and w_1, the first components of $\boldsymbol{z}$ and $\boldsymbol{w}$, to* 1.

2. *For $s = 2, 3, \ldots, d-1, d$, do the following:*

(a) *Find* $z_s \in \left\{1, 2, \ldots, \frac{p-1}{2}\right\}$ *to minimize*

$$
\begin{aligned}
&\hat{\theta}_{p,q,s}\left((z_1,\ldots,z_{s-1}),(w_1,\ldots,w_{s-1});z_s\right)\\
&= \left(\beta_s + \tfrac{\gamma_s}{3}\right)\hat{e}^2_{p,q,s-1}\left((z_1,\ldots,z_{s-1}),(w_1,\ldots,w_{s-1})\right)\\
&\quad + \frac{\gamma_s}{6pq}\prod_{j=1}^{s-1}\left(\beta_j + \tfrac{\gamma_j}{2}\right)\\
&\quad + \frac{\gamma_s}{pq}\sum_{i=1}^{p-1}\left[\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right)B_2\left(\left\{\tfrac{iz_s}{p}\right\}\right)\right]\\
&\quad - \frac{\gamma_s}{6pq^2}\sum_{k=1}^{q-1}\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right)\\
&\quad + \frac{\gamma_s}{pq}\sum_{i=1}^{p-1}\sum_{k=1}^{q-1}\left[\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right)\right.\\
&\qquad\qquad \left.\times\left(\tfrac{1}{q(q-1)}B_2\left(\left\{\tfrac{qiz_s}{p}\right\}\right) - \tfrac{1}{q-1}B_2\left(\left\{\tfrac{iz_s}{p}\right\}\right)\right)\right].
\end{aligned}
$$

(b) *Find* $w_s \in \{1, 2, \ldots, q-1\}$ *to minimize*

$$
\begin{aligned}
&\hat{e}^2_{p,q,s}\left((z_1,\ldots,z_s),(w_1,\ldots,w_s)\right)\\
&= -\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{3}\right)\\
&\quad + \frac{1}{pq}\sum_{i=0}^{p-1}\sum_{k=0}^{q-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right).
\end{aligned}
$$

8.2.2 An improved bound

The following theorem shows that with some minor restrictions on p and q, the randomly shifted rank-1 lattice rule constructed by Algorithm 8.7 has a square worst-case error smaller than the QMC mean (see Lemma 2.17).

Theorem 8.8 *Let* $n = pq$ *where* p *and* q *are two distinct prime numbers such that*

$$p,\, q \geq 2\exp\left(\frac{1}{6}\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j}\right).$$

Suppose there exist $\boldsymbol{z} \in \mathbb{Z}_p^d$ *and* $\boldsymbol{w} \in \mathbb{Z}_q^d$ *such that*

$$\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}) \leq E_{n,d}, \text{ where } E_{n,d} = \frac{1}{n}\left(\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{2}\right) - \prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right)\right)$$

is the QMC mean. Then there exist $z_{d+1} \in \mathbb{Z}_p$ and $w_{d+1} \in \mathbb{Z}_q$ such that

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \le E_{n,d+1}.$$

A pair (z_{d+1}, w_{d+1}) satisfying this bound can be found by first minimizing $\hat{\theta}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}; z_{d+1})$ over all $z_{d+1} \in \mathbb{Z}_p$ and then (with this z_{d+1} fixed) minimizing $\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right)$ over all $w_{d+1} \in \mathbb{Z}_q$. Moreover, we have $\hat{e}^2_{p,q,1}(z_1, w_1) \le E_{n,1}$ for all $z_1 \in \mathbb{Z}_p$ and $w_1 \in \mathbb{Z}_q$.

Proof. We have from Theorem 8.5 that

$$\hat{m}_{p,q,d+1}(\boldsymbol{z}, \boldsymbol{w}) \le \left(\beta_{d+1} + \tfrac{\gamma_{d+1}}{3}\right) \hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w}) + \frac{\gamma_{d+1}}{6pq} \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{2}\right) + \frac{\gamma_{d+1}}{6p^2q^2} \times G,$$

where

$$\begin{aligned} G &= \sum_{i=1}^{p-1} \sum_{k=1}^{q-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right) \right. \\ &\quad \left. - \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right) - \prod_{j=1}^{d} \left(\beta_j + \gamma_j \left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right) \right]. \end{aligned}$$

Using Lemma 3.5, we can write G as

$$\begin{aligned} G &= \sum_{i=1}^{p-1} \sum_{k=1}^{q-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left[\prod_{j \notin \mathfrak{u}} \left(\beta_j + \tfrac{\gamma_j}{3}\right) \prod_{j \in \mathfrak{u}} \gamma_j \right. \\ &\quad \left. \times \left(\prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) - \prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) - \prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) \right) \right] \\ &= -(p-1)(q-1) \prod_{j=1}^{d} \left(\beta_j + \tfrac{\gamma_j}{3}\right) + \sum_{\emptyset \ne \mathfrak{u} \subseteq \mathcal{D}} \left[\prod_{j \notin \mathfrak{u}} \left(\beta_j + \tfrac{\gamma_j}{3}\right) \prod_{j \in \mathfrak{u}} \gamma_j \times H(\mathfrak{u}) \right], \end{aligned}$$

where

$$\begin{aligned} H(\mathfrak{u}) &= \sum_{i=1}^{p-1} \sum_{k=1}^{q-1} \left(\prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) - \prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) - \prod_{j \in \mathfrak{u}} B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) \right) \\ &= \frac{1}{(2\pi^2)^{|\mathfrak{u}|}} \sum_{i=1}^{p-1} \sum_{k=1}^{q-1} \left[\prod_{j \in \mathfrak{u}} \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h (iz_j/p + kw_j/q)}}{h^2} \right. \\ &\quad \left. - \prod_{j \in \mathfrak{u}} \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h i z_j/p}}{h^2} - \prod_{j \in \mathfrak{u}} \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k w_j/q}}{h^2} \right]. \end{aligned}$$

Now let $\boldsymbol{z}_{\mathrm{u}}$ denote the $|\mathrm{u}|$-dimensional vector containing those components of $\boldsymbol{z}$ whose indices belong to u. Then we can rewrite $H(\mathrm{u})$ as

$$\begin{aligned} H(\mathrm{u}) &= \frac{1}{(2\pi^2)^{|\mathrm{u}|}} \sum_{i=1}^{p-1}\sum_{k=1}^{q-1} \Bigg[\sum_{\boldsymbol{h}\in\mathbb{Z}^{|\mathrm{u}|}}{}' \frac{e^{2\pi \mathrm{i}(i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p + k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q)}}{h_1^2\cdots h_{|\mathrm{u}|}^2} \\ &\qquad - \sum_{\boldsymbol{h}\in\mathbb{Z}^{|\mathrm{u}|}}{}' \frac{e^{2\pi \mathrm{i} i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p}}{h_1^2\cdots h_{|\mathrm{u}|}^2} - \sum_{\boldsymbol{h}\in\mathbb{Z}^{|\mathrm{u}|}}{}' \frac{e^{2\pi \mathrm{i} k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q}}{h_1^2\cdots h_{|\mathrm{u}|}^2}\Bigg] \\ &= \frac{1}{(2\pi^2)^{|\mathrm{u}|}} \sum_{\boldsymbol{h}\in\mathbb{Z}^{|\mathrm{u}|}}{}' \Bigg[\frac{1}{h_1^2\cdots h_{|\mathrm{u}|}^2} \sum_{i=1}^{p-1}\sum_{k=1}^{q-1} \Big(e^{2\pi \mathrm{i}(i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p + k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q)} \\ &\qquad - e^{2\pi \mathrm{i} i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p} - e^{2\pi \mathrm{i} k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q}\Big)\Bigg]. \end{aligned}$$

It can be shown that

$$\begin{aligned} &\sum_{i=1}^{p-1}\sum_{k=1}^{q-1} \Big(e^{2\pi \mathrm{i}(i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p + k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q)} - e^{2\pi \mathrm{i} i\boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}}/p} - e^{2\pi \mathrm{i} k\boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}}/q}\Big) \\ &= \begin{cases} p+q-1, & \text{if } \boldsymbol{h}\cdot\boldsymbol{z}_{\mathrm{u}} \not\equiv 0 \,(\mathrm{mod}\, p) \text{ and } \boldsymbol{h}\cdot\boldsymbol{w}_{\mathrm{u}} \not\equiv 0 \,(\mathrm{mod}\, q), \\ -(p-1)(q-1) \le p+q-1, & \text{otherwise.} \end{cases} \end{aligned}$$

Thus

$$\begin{aligned} H(\mathrm{u}) &\le \frac{p+q-1}{(2\pi^2)^{|\mathrm{u}|}} \sum_{\boldsymbol{h}\in\mathbb{Z}^{|\mathrm{u}|}}{}' \frac{1}{h_1^2\cdots h_{|\mathrm{u}|}^2} \\ &= \frac{p+q-1}{(2\pi^2)^{|\mathrm{u}|}} \left(2\zeta(2)\right)^{|\mathrm{u}|} = \frac{p+q-1}{(2\pi^2)^{|\mathrm{u}|}} \left(\frac{2\pi^2}{6}\right)^{|\mathrm{u}|} = \frac{p+q-1}{6^{|\mathrm{u}|}}, \end{aligned}$$

which leads to

$$\begin{aligned} G &\le -(p-1)(q-1)\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right) \\ &\qquad + (p+q-1)\sum_{\emptyset\ne\mathrm{u}\subseteq\mathcal{D}} \left[\prod_{j\notin\mathrm{u}}\left(\beta_j + \tfrac{\gamma_j}{3}\right)\prod_{j\in\mathrm{u}}\left(\tfrac{\gamma_j}{6}\right)\right] \\ &= -(p-1)(q-1)\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right) \\ &\qquad + (p+q-1)\left(\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{2}\right) - \prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right)\right) \\ &= -pq\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{3}\right) + (p+q-1)\prod_{j=1}^{d}\left(\beta_j + \tfrac{\gamma_j}{2}\right), \end{aligned}$$

and in turn we have

$$\begin{aligned}
\hat{m}_{p,q,d+1}(\boldsymbol{z},\boldsymbol{w}) &\le \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}) + \frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right) \\
&\quad + \frac{\gamma_{d+1}}{6p^2q^2}\left(-pq\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right)+(p+q-1)\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)\right) \\
&= \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}) \\
&\quad + \frac{\gamma_{d+1}}{6pq}\left(1+\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right) - \frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right).
\end{aligned}$$

Using the assumption that $\hat{e}^2_{p,q,d}(\boldsymbol{z},\boldsymbol{w}) \le E_{n,d}$, we have

$$\begin{aligned}
\hat{m}_{p,q,d+1}(\hat{\boldsymbol{z}},\hat{\boldsymbol{w}}) &\le \left(\beta_{d+1}+\tfrac{\gamma_{d+1}}{3}\right)\times\frac{1}{pq}\left(\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)-\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right)\right) \\
&\quad + \frac{\gamma_{d+1}}{6pq}\left(1+\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right) - \frac{\gamma_{d+1}}{6pq}\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right) \\
&= \frac{1}{pq}\left(\prod_{j=1}^{d+1}\left(\beta_j+\tfrac{\gamma_j}{2}\right)-\prod_{j=1}^{d+1}\left(\beta_j+\tfrac{\gamma_j}{3}\right)\right)+\frac{\gamma_{d+1}}{6pq}\times T,
\end{aligned}$$

where

$$T = \left(\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)-\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right).$$

Now consider

$$R = \frac{\left(\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{2}\right)}{\prod_{j=1}^{d}\left(\beta_j+\tfrac{\gamma_j}{3}\right)} = \left(\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\prod_{j=1}^{d}\left(1+\tfrac{\gamma_j}{6\beta_j+2\gamma_j}\right).$$

Since

$$p,\, q \ge 2\exp\left(\frac{1}{6}\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j}\right),$$

we have

$$R = \left(\tfrac{1}{p}+\tfrac{1}{q}-\tfrac{1}{pq}\right)\exp\left(\sum_{j=1}^{d}\log\left(1+\tfrac{\gamma_j}{6\beta_j+2\gamma_j}\right)\right) \le \left(\tfrac{1}{p}+\tfrac{1}{q}\right)\exp\left(\tfrac{1}{6}\sum_{j=1}^{\infty}\tfrac{\gamma_j}{\beta_j}\right) \le 1.$$

Thus, $T \le 0$ and this leads to

$$\hat{m}_{p,q,d+1}(\hat{\boldsymbol{z}},\hat{\boldsymbol{w}}) \le \frac{1}{pq}\left(\prod_{j=1}^{d+1}\left(\beta_j+\tfrac{\gamma_j}{2}\right)-\prod_{j=1}^{d+1}\left(\beta_j+\tfrac{\gamma_j}{3}\right)\right) = E_{n,d+1}.$$

Hence we can choose a pair (z_{d+1}, w_{d+1}) following the proof of Theorem 8.6 such that

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \le E_{n,d+1}.$$

In one dimension, $E_{n,1} = \frac{\gamma_1}{6n}$ and we have from the proof of Theorem 8.6 that $\hat{e}^2_{p,q,1}(z_1, w_1) = \hat{e}^2_{p,q,1}(1,1) = \frac{\gamma_1}{6p^2q^2}$. Thus $\hat{e}^2_{p,q,1}(z_1, w_1) \le E_{n,1}$ for all $z_1 \in \mathbb{Z}_p$ and $w_1 \in \mathbb{Z}_q$. This completes the proof. □

The condition of

$$p,\ q \ge 2\exp\left(\frac{1}{6}\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j}\right)$$

is not unreasonable at all. For example, for $\beta_j = 1$ and $\gamma_j = 0.5^j$ we need $p, q \ge 3$; for $\beta_j = 1$ and $\gamma_j = 0.9^j$ we need $p, q \ge 9$; for $\beta_j = 1$ and $\gamma_j = 1/j^2$ we need $p, q \ge 3$.

8.2.3 A possible construction in practice

The cost for the component-by-component construction in Algorithm 8.7 is $O(n(p+q)d^2)$ operations and for p and q roughly the same, the cost is $O(n^{1.5}d^2)$ operations. Here we propose a construction with cost $O(nd^2)$ operations which seems to work in practice (as our numerical experiments will show in Chapter 10), but we do not have a theoretical justification yet.

We construct $\boldsymbol{z}$ component-by-component by minimizing the mean $\hat{\Theta}_{p,q,d}(\boldsymbol{z})$, and construct $\boldsymbol{w}$ component-by-component by minimizing the mean $\hat{\Omega}_{p,q,d}(\boldsymbol{w})$. (The expressions for these means can be found in Theorem 8.2.) We can then evaluate $\hat{e}^2_{p,q,d}(\boldsymbol{z}, \boldsymbol{w})$ to see if it is bounded by the QMC mean $E_{n,d}$. The costs for the construction of $\boldsymbol{z}$ and $\boldsymbol{w}$ will be $O(p^2d^2)$ and $O(q^2d^2)$ operations respectively, and it requires $O(pqd)$ operations to check the bound. (See Chapter 10 later for results of numerical experiments.)

Because of the symmetric property of B_2, it is clear that

$$\hat{\Theta}_{p,q,d+1}(\boldsymbol{z}, z_{d+1}) = \hat{\Theta}_{p,q,d+1}(\boldsymbol{z}, p - z_{d+1}),$$

and

$$\hat{\Omega}_{p,q,d+1}(\boldsymbol{w}, w_{d+1}) = \hat{\Omega}_{p,q,d+1}(\boldsymbol{w}, q - w_{d+1}).$$

Thus the searches of z_{d+1} and w_{d+1} can be restricted to the sets $\{1, 2, \ldots, \frac{p-1}{2}\}$ and $\{1, 2, \ldots, \frac{q-1}{2}\}$ respectively. Now since

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) = \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, p - z_{d+1}), (\boldsymbol{w}, q - w_{d+1})\right),$$

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, q - w_{d+1})\right) = \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, p - z_{d+1}), (\boldsymbol{w}, w_{d+1})\right),$$

but in general

$$\hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, w_{d+1})\right) \neq \hat{e}^2_{p,q,d+1}\left((\boldsymbol{z}, z_{d+1}), (\boldsymbol{w}, q - w_{d+1})\right),$$

we evaluate both these two square errors and see which is the smaller of the two.

Algorithm 8.9 [Separate Search]

Given two distinct prime numbers p and q:

1. *Set z_1 and w_1, the first components of $\boldsymbol{z}$ and $\boldsymbol{w}$, to 1.*

2. *For $s = 2, 3, \ldots, d-1, d$, do the following:*

   (a) *Find $z_s \in \{1, 2, \ldots, \frac{p-1}{2}\}$ to minimize*

$$\begin{aligned}
\hat{\Theta}_{p,q,s}(z_1, \ldots, z_s) &= -\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{3}\right) + \frac{1}{pq}\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{2}\right) \\
&\quad + \frac{q-1}{pq}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6q}\right)\right) \\
&\quad + \frac{1}{pq}\sum_{i=1}^{p-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right) \\
&\quad + \frac{q-1}{pq}\sum_{i=1}^{p-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[\tfrac{1}{q(q-1)}B_2\left(\left\{\tfrac{qiz_j}{p}\right\}\right)\right.\right. \\
&\qquad \left.\left. - \tfrac{1}{q-1}B_2\left(\left\{\tfrac{iz_j}{p}\right\}\right) + \tfrac{1}{3}\right]\right).
\end{aligned}$$

(b) *Find* $w_s \in \left\{1, 2, \ldots, \frac{q-1}{2}\right\}$ *to minimize*

$$\begin{aligned}\hat{\Omega}_{p,q,s}(w_1,\ldots,w_s) &= -\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{3}\right) + \frac{1}{pq}\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{2}\right) \\ &+ \frac{p-1}{pq}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left(\tfrac{1}{3} - \tfrac{1}{6p}\right)\right) \\ &+ \frac{1}{pq}\sum_{k=1}^{q-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right) \\ &+ \frac{p-1}{pq}\sum_{k=1}^{q-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[\tfrac{1}{p(p-1)}B_2\left(\left\{\tfrac{pkw_j}{q}\right\}\right)\right.\right. \\ &\qquad\left.\left. - \tfrac{1}{p-1}B_2\left(\left\{\tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right).\end{aligned}$$

(c) *If*

$$\begin{aligned}&\hat{e}^2_{p,q,s}\left((z_1,\ldots,z_s),(w_1,\ldots,q-w_s)\right) \\ &= -\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{3}\right) \\ &+ \frac{1}{pq}\sum_{i=0}^{p-1}\sum_{k=0}^{q-1}\left[\prod_{j=1}^{s-1}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right)\right. \\ &\qquad\left. \times\left(\beta_s + \gamma_s\left[B_2\left(\left\{\tfrac{iz_s}{p} + \tfrac{k(q-w_s)}{q}\right\}\right) + \tfrac{1}{3}\right]\right)\right],\end{aligned}$$

is smaller than

$$\begin{aligned}&\hat{e}^2_{p,q,s}\left((z_1,\ldots,z_s),(w_1,\ldots,w_s)\right) \\ &= -\prod_{j=1}^{s}\left(\beta_j + \tfrac{\gamma_j}{3}\right) \\ &+ \frac{1}{pq}\sum_{i=0}^{p-1}\sum_{k=0}^{q-1}\prod_{j=1}^{s}\left(\beta_j + \gamma_j\left[B_2\left(\left\{\tfrac{iz_j}{p} + \tfrac{kw_j}{q}\right\}\right) + \tfrac{1}{3}\right]\right),\end{aligned}$$

change w_s *to* $q - w_s$.

Chapter 9

Component-by-component Constructions Achieve the Optimal Rate of Convergence

It is known from the analysis by Sloan and Woźniakowski [36] that under appropriate conditions on the weights, the optimal rate of convergence for multiple integration in weighted Korobov spaces with parameter $\alpha > 1$ is $O(n^{-\frac{\alpha}{2}+\delta})$ for any $\delta > 0$, and the optimal rate in weighted Sobolev spaces is $O(n^{-1+\delta})$ for any $\delta > 0$. However, their work did not show how rules achieving these rates of convergence could be constructed. The existing theory behind the component-by-component constructions given by Algorithms 3.10 and 6.4 indicate that the rules constructed achieve $O(n^{-\frac{1}{2}})$ convergence. Here we present theorems which show that those lattice rules constructed in fact achieve the optimal rate of convergence in the corresponding weighted function spaces.

9.1 Constructing rank-1 lattice rules with error $O(n^{-\alpha/2+\delta})$ in weighted Korobov spaces

In this section we look into the construction of rank-1 lattice rules given by Algorithm 3.10 in Chapter 3 where for simplicity n was chosen to be a prime number. We see from Theorem 3.8 and Corollary 3.9 that the generating vector $\boldsymbol{z}$ constructed by Algorithm 3.10 satisfies

$$e_{n,d}^2(\boldsymbol{z}) \leq \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + 4\gamma_j \zeta(\alpha)\right),$$

and when

$$\sum_{j=1}^{\infty} \frac{\gamma_j}{\beta_j} < \infty,$$

the rules are guaranteed to achieve $O(n^{-\frac{1}{2}})$ convergence, with the implied constant independent of d.

It follows from a generalization of [36] that the optimal rate of convergence for QMC rules in weighted Korobov spaces is $O(n^{-\frac{\alpha}{2}+\delta})$ for any $\delta > 0$, with the implied constant independent of d, which leads to the ε-exponent of strong tractability being equal to $\frac{2}{\alpha}$. Further, there exist rank-1 lattice rules that achieve this optimal rate of convergence when the weights satisfy

$$\sum_{j=1}^{\infty} \left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}} < \infty,$$

for any $\delta > 0$. Here we show that the rules constructed by Algorithm 3.10 in fact achieve this optimal rate of convergence.

9.1.1 An improved bound for the construction

Theorem 9.1 and Corollary 9.2 below give the theoretical foundation for Algorithm 3.10 using a different upper bound to that of Theorem 3.8 and Corollary 3.9. The proofs for these results make use of Jensen's inequality extensively. In its most general form, Jensen's inequality (see Theorem 19 of [7]) states that if $\{a_k\}$ is a sequence of positive numbers, then

$$\left(\sum a_k^p\right)^{\frac{1}{p}} \leq \left(\sum a_k^q\right)^{\frac{1}{q}} \quad \text{for } 0 < q \leq p.$$

We apply this inequality to the case where $p = 1$ and $q = \lambda$, that is,

$$\sum a_k \leq \left(\sum a_k^\lambda\right)^{\frac{1}{\lambda}} \quad \text{for } 0 < \lambda \leq 1. \tag{9.1}$$

Theorem 9.1 *Let n be a prime number and let $\frac{1}{\alpha} < \lambda \leq 1$. Suppose there exists $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that*

$$e_{n,d}^2(\boldsymbol{z}) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}}.$$

Then there exists $z_{d+1} \in \mathbb{Z}_n$ such that

$$e_{n,d+1}^2(\boldsymbol{z}, z_{d+1}) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d+1} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}}.$$

Proof. It follows from Lemma 3.1 that

$$e_{n,d+1}^2(\boldsymbol{z}, z_{d+1}) = \beta_{d+1} e_{n,d}^2(\boldsymbol{z}) + \psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}),$$

where

$$\begin{aligned} &\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \\ &:= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j \sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z_j / n}}{|h|^\alpha} \right) \left(\sum_{h=-\infty}^{\infty}{}' \frac{e^{2\pi i h k z_{d+1} / n}}{|h|^\alpha} \right) \right]. \end{aligned}$$

Later we shall prove the following:

(i) For given α, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and $\boldsymbol{z}$, there exists $z_{d+1} = z_{d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z})$ such that

$$\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \leq \frac{4\gamma_{d+1}\zeta(\alpha)}{n} \prod_{j=1}^{d} \left(\beta_j + 2\gamma_j \zeta(\alpha)\right).$$

(ii) We have

$$\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \leq \left(\psi_{n,d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z}, z_{d+1})\right)^{\frac{1}{\lambda}},$$

where $\boldsymbol{\beta}^\lambda = \{\beta_j^\lambda\}$ and $\boldsymbol{\gamma}^\lambda = \{\gamma_j^\lambda\}$.

We see from (i) with α replaced by $\alpha\lambda$, $\boldsymbol{\beta}$ replaced by $\boldsymbol{\beta}^\lambda$, and $\boldsymbol{\gamma}$ replaced by $\boldsymbol{\gamma}^\lambda$ that there exists $z_{d+1} = z_{d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z})$ such that

$$\psi_{n,d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z}, z_{d+1}) \le \frac{4\gamma_{d+1}^\lambda \zeta(\alpha\lambda)}{n} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right).$$

For this $z_{d+1} = z_{d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z})$, it then follows from (ii) that

$$\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \le \left(\frac{4\gamma_{d+1}^\lambda \zeta(\alpha\lambda)}{n}\right)^{\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}}.$$

Thus this $z_{d+1} = z_{d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z})$ satisfies

$$\begin{aligned}
e_{n,d+1}^2(\boldsymbol{z}, z_{d+1}) &\le \beta_{d+1} \times 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}} \\
&\quad + \left(\frac{4\gamma_{d+1}^\lambda \zeta(\alpha\lambda)}{n}\right)^{\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}} \\
&= \left(\beta_{d+1} + 2^{\frac{1}{\lambda}} \gamma_{d+1} \zeta(\alpha\lambda)^{\frac{1}{\lambda}}\right) \times 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}} \\
&\le \left(\beta_{d+1}^\lambda + 2\gamma_{d+1}^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}} \times 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}} \\
&= 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d+1} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}},
\end{aligned}$$

where in the second to last step we have used Jensen's inequality (9.1) in the first factor. Hence the theorem is proved if we can prove (i) and (ii).

Proof of (i): Let $T_\alpha(k, n)$ be as given in Lemma 3.2. We form an average of $\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1})$ over the possible values of z_{d+1}:

$$\begin{aligned}
\Psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}) &:= \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} \psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \\
&= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j {\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i h k z_j / n}}{|h|^\alpha} \right) T_\alpha(k, n) \right] \\
&\le \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \gamma_j {\sum_{h=-\infty}^{\infty}}' \frac{1}{|h|^\alpha} \right) |T_\alpha(k, n)| \right] \\
&= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} |T_\alpha(k, n)| \prod_{j=1}^{d} \left(\beta_j + 2\gamma_j \zeta(\alpha)\right).
\end{aligned}$$

It then follows from Lemma 3.2 that

$$\sum_{k=0}^{n-1} |T_\alpha(k,n)| = |T_\alpha(0,n)| + \sum_{k=1}^{n-1} |T_\alpha(k,n)| = 2\zeta(\alpha)(2 - n^{1-\alpha}) \leq 4\zeta(\alpha).$$

Hence

$$\Psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}) \leq \frac{4\gamma_{d+1}\zeta(\alpha)}{n} \prod_{j=1}^{d} \left(\beta_j + 2\gamma_j\zeta(\alpha)\right),$$

and thus there exists $z_{d+1} = z_{d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z})$ such that

$$\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \leq \Psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}) \leq \frac{4\gamma_{d+1}\zeta(\alpha)}{n} \prod_{j=1}^{d} \left(\beta_j + 2\gamma_j\zeta(\alpha)\right).$$

Proof of (ii): Let

$$r(\alpha, \beta, \gamma, h) := \begin{cases} \beta^{-1}, & \text{if } h = 0, \\ \gamma^{-1}|h|^\alpha, & \text{if } h \neq 0. \end{cases}$$

We can write

$$\begin{aligned} &\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \\ &= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \left[\prod_{j=1}^{d} \left(\sum_{h=-\infty}^{\infty} \frac{e^{2\pi i hkz_j/n}}{r(\alpha, \beta_j, \gamma_j, h)} \right) \left({\sum_{h=-\infty}^{\infty}}' \frac{e^{2\pi i hkz_{d+1}/n}}{|h|^\alpha} \right) \right] \\ &= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \sum_{\substack{\boldsymbol{h} \in \mathbb{Z}^{d+1} \\ h_{d+1} \neq 0}} \frac{e^{2\pi i k \boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1})/n}}{|h_{d+1}|^\alpha \prod_{j=1}^{d} r(\alpha, \beta_j, \gamma_j, h_j)}. \end{aligned}$$

If $\boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1})$ is not a multiple of n, then

$$\sum_{k=0}^{n-1} e^{2\pi i k \boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1})/n} = \sum_{k=0}^{n-1} \left(e^{2\pi i \boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1})/n}\right)^k = 0.$$

Thus

$$\begin{aligned} &\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \\ &= \frac{\gamma_{d+1}}{n} \sum_{k=0}^{n-1} \sum_{\substack{\boldsymbol{h} \in \mathbb{Z}^{d+1} \\ h_{d+1} \neq 0 \\ \boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1}) \equiv 0 \pmod n}} \frac{1}{|h_{d+1}|^\alpha \prod_{j=1}^{d} r(\alpha, \beta_j, \gamma_j, h_j)} \\ &= \sum_{\substack{\boldsymbol{h} \in \mathbb{Z}^{d+1} \\ h_{d+1} \neq 0 \\ \boldsymbol{h} \cdot (\boldsymbol{z}, z_{d+1}) \equiv 0 \pmod n}} \left(\gamma_{d+1} |h_{d+1}|^{-\alpha} \prod_{j=1}^{d} r(\alpha, \beta_j, \gamma_j, h_j)^{-1} \right). \end{aligned} \tag{9.2}$$

Applying Jensen's inequality (9.1) to (9.2) and then using the property

$$\begin{aligned} r(\alpha,\beta,\gamma,h)^\lambda &= \begin{cases} \beta^{-\lambda}, & \text{if } h = 0, \\ \gamma^{-\lambda}|h|^{\alpha\lambda}, & \text{if } h \neq 0, \end{cases} \\ &= r(\alpha\lambda, \beta^\lambda, \gamma^\lambda, h), \end{aligned}$$

we obtain

$$\begin{aligned} &\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \\ &\leq \left(\sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^{d+1} \\ h_{d+1}\neq 0 \\ \boldsymbol{h}\cdot(\boldsymbol{z},z_{d+1})\equiv 0 (\bmod n)}} \left(\gamma_{d+1}^\lambda |h_{d+1}|^{-\alpha\lambda} \prod_{j=1}^d r(\alpha, \beta_j, \gamma_j, h_j)^{-\lambda} \right) \right)^{\frac{1}{\lambda}} \\ &= \left(\sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^{d+1} \\ h_{d+1}\neq 0 \\ \boldsymbol{h}\cdot(\boldsymbol{z},z_{d+1})\equiv 0 (\bmod n)}} \left(\gamma_{d+1}^\lambda |h_{d+1}|^{-\alpha\lambda} \prod_{j=1}^d r(\alpha\lambda, \beta_j^\lambda, \gamma_j^\lambda, h_j)^{-1} \right) \right)^{\frac{1}{\lambda}}. \end{aligned}$$

Note that the sum inside the brackets on the right-hand side is exactly (9.2) with α replaced by $\alpha\lambda$, $\boldsymbol{\beta}$ replaced by $\boldsymbol{\beta}^\lambda$, and $\boldsymbol{\gamma}$ replaced by $\boldsymbol{\gamma}^\lambda$. Thus

$$\psi_{n,d+1}(\alpha, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{z}, z_{d+1}) \leq \left(\psi_{n,d+1}(\alpha\lambda, \boldsymbol{\beta}^\lambda, \boldsymbol{\gamma}^\lambda, \boldsymbol{z}, z_{d+1})\right)^{\frac{1}{\lambda}}.$$

This completes the proof. □

Theorem 9.1 shows that there exists a value of z_{d+1} for which the square worst-case error satisfies the desired bound. Then clearly the value of z_{d+1} which minimizes the square worst-case error also satisfies the bound, and hence we find z_{d+1} this way. This is the content of Corollary 9.2 below.

Corollary 9.2 *Let n be a prime number. We can construct $\boldsymbol{z} \in \mathbb{Z}_n^d$ component-by-component such that for all $s = 1, \ldots, d$,*

$$e_{n,s}^2(z_1, \ldots, z_s) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^s \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}},$$

for all λ satisfying $\frac{1}{\alpha} < \lambda \leq 1$. We can set $z_1 = 1$, and for s satisfying $2 \leq s \leq d$, each z_s can be found by minimizing $e_{n,s}^2(z_1, \ldots, z_s)$ over the set $\mathbb{Z}_n$.

Proof. In one dimension, it follows from (3.2) that

$$e_{n,1}^2(z_1) = e_{n,1}^2(1) = \frac{2\gamma_1\zeta(\alpha)}{n^\alpha}.$$

For any λ satisfying $\frac{1}{\alpha} < \lambda \le 1$, we have

$$\frac{2\gamma_1\zeta(\alpha)}{n^\alpha} \le 2^{\frac{1}{\lambda}} n^{-\alpha} \left(\beta_1 + 2\gamma_1\zeta(\alpha)\right) \le 2^{\frac{1}{\lambda}} n^{-\alpha} \left(\beta_1^\lambda + 2^\lambda \gamma_1^\lambda [\zeta(\alpha)]^\lambda\right)^{\frac{1}{\lambda}},$$

where this second inequality follows when we apply Jensen's inequality (9.1) to the factor $(\beta_1 + 2\gamma_1\zeta(\alpha))$. Clearly $n^{-\alpha} < n^{-\frac{1}{\lambda}}$, $2^\lambda \le 2$, and by Jensen's inequality (9.1),

$$[\zeta(\alpha)]^\lambda = \left[\sum_{h=1}^{\infty} \frac{1}{h^\alpha}\right]^\lambda \le \left[\left(\sum_{h=1}^{\infty} \frac{1}{h^{\alpha\lambda}}\right)^{\frac{1}{\lambda}}\right]^\lambda = \zeta(\alpha\lambda).$$

Thus we have for all z_1,

$$e_{n,1}^2(z_1) = \frac{2\gamma_1\zeta(\alpha)}{n^\alpha} \le 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \left(\beta_1^\lambda + 2\gamma_1^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}}.$$

Note that this bound holds for arbitrary λ satisfying $\frac{1}{\alpha} < \lambda \le 1$.

For each $s = 2, \ldots, d$, it follows inductively from Theorem 9.1 with $d = s-1$ that z_s can be found by minimizing $e_{n,s}^2(z_1, \ldots, z_s)$ over the set $\mathbb{Z}_n$ and the bound

$$e_{n,s}^2(z_1, \ldots, z_s) \le 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{s} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{\frac{1}{\lambda}},$$

holds for arbitrary λ satisfying $\frac{1}{\alpha} < \lambda \le 1$. This completes the proof. □

Corollary 9.2 leads us to our existing algorithm, Algorithm 3.10. We emphasize here that the generating vector $\boldsymbol{z}$ constructed by the algorithm is independent of λ.

9.1.2 The construction achieves the optimal rate of convergence

Theorem 9.3 below asserts that with the new upper bound given by Theorem 9.1 and Corollary 9.2, the rules constructed by Algorithm 3.10 achieve the optimal rate of convergence.

Theorem 9.3 *Let n be a prime number and let $\boldsymbol{z}$ be constructed component-by-component as in Algorithm 3.10. Then this $\boldsymbol{z}$ satisfies*

$$e_{n,d}(\boldsymbol{z}) \le C_d(\delta)\, n^{-\frac{\alpha}{2}+\delta} e_{0,d}, \quad \textit{for all} \quad 0 < \delta \le \tfrac{\alpha-1}{2},$$

where

$$C_d(\delta) = 2^{\frac{\alpha}{2}-\delta} \prod_{j=1}^{d} \left[1 + 2 \left(\frac{\gamma_j}{\beta_j} \right)^{\frac{1}{\alpha-2\delta}} \zeta\left(\frac{\alpha}{\alpha - 2\delta} \right) \right]^{\frac{\alpha}{2}-\delta} \quad \textit{and} \quad e_{0,d} = \prod_{j=1}^{d} \beta_j^{\frac{1}{2}}.$$

Moreover, if

$$\sum_{j=1}^{\infty} \left(\frac{\gamma_j}{\beta_j} \right)^{\frac{1}{\alpha-2\delta}} < \infty,$$

then

$$C_d(\delta) \le C_\infty(\delta) < \infty,$$

that is, $e_{n,d}(\boldsymbol{z})$ is $O(n^{-\frac{\alpha}{2}+\delta})$ for $\delta > 0$, independently of d, with the ε-exponent of strong tractability being $\frac{2}{\alpha}$.

Proof. It follows from Corollary 9.2 that $\boldsymbol{z}$ constructed by Algorithm 3.10 satisfies

$$\begin{aligned} e_{n,d}(\boldsymbol{z}) &\le 2^{\frac{1}{2\lambda}} n^{-\frac{1}{2\lambda}} \prod_{j=1}^{d} \left(\beta_j^\lambda + 2\gamma_j^\lambda \zeta(\alpha\lambda) \right)^{\frac{1}{2\lambda}} \\ &= 2^{\frac{1}{2\lambda}} n^{-\frac{1}{2\lambda}} \prod_{j=1}^{d} \left(1 + 2 \left(\frac{\gamma_j}{\beta_j} \right)^{\lambda} \zeta(\alpha\lambda) \right)^{\frac{1}{2\lambda}} \prod_{j=1}^{d} \beta_j^{\frac{1}{2}}, \quad \text{for all } \tfrac{1}{\alpha} < \lambda \le 1. \end{aligned}$$

Now with the substitution of

$$-\frac{\alpha}{2} + \delta = -\frac{1}{2\lambda},$$

we obtain

$$e_{n,d}(\boldsymbol{z}) \le C_d(\delta)\, n^{-\frac{\alpha}{2}+\delta} e_{0,d}, \quad \text{for all } 0 < \delta \le \tfrac{\alpha-1}{2},$$

where

$$C_d(\delta) = 2^{\frac{\alpha}{2}-\delta} \prod_{j=1}^{d} \left[1 + 2 \left(\frac{\gamma_j}{\beta_j} \right)^{\frac{1}{\alpha-2\delta}} \zeta\left(\frac{\alpha}{\alpha - 2\delta} \right) \right]^{\frac{\alpha}{2}-\delta} \le C_\infty(\delta).$$

We have

$$\begin{aligned}
C_\infty(\delta) &= 2^{\frac{\alpha}{2}-\delta}\prod_{j=1}^{\infty}\left[1+2\left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}}\zeta\left(\frac{\alpha}{\alpha-2\delta}\right)\right]^{\frac{\alpha}{2}-\delta} \\
&= 2^{\frac{\alpha}{2}-\delta}\exp\left(\left(\frac{\alpha}{2}-\delta\right)\sum_{j=1}^{\infty}\log\left(1+2\left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}}\zeta\left(\frac{\alpha}{\alpha-2\delta}\right)\right)\right) \\
&\leq 2^{\frac{\alpha}{2}-\delta}\exp\left(\left(\frac{\alpha}{2}-\delta\right)\sum_{j=1}^{\infty}\left[2\left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}}\zeta\left(\frac{\alpha}{\alpha-2\delta}\right)\right]\right) \\
&= 2^{\frac{\alpha}{2}-\delta}\exp\left((\alpha-2\delta)\,\zeta\left(\frac{\alpha}{\alpha-2\delta}\right)\sum_{j=1}^{\infty}\left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}}\right),
\end{aligned}$$

where in the second to last step we have used the fact that $\log(1+x) \leq x$ for $x \geq 0$. It is clear from this expression that for $\delta > 0$, $C_\infty(\delta) < \infty$ if

$$\sum_{j=1}^{\infty}\left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{\alpha-2\delta}} < \infty.$$

This completes the proof. □

9.2 Constructing randomly shifted rank-1 lattice rules with error $O(n^{-1+\delta})$ in weighted Sobolev spaces

Now we recall from Chapter 6 that the generating vector $\boldsymbol{z}$ for a randomly shifted rank-1 lattice rule can be constructed by Algorithm 6.4, and when the weights satisfy

$$\sum_{j=1}^{\infty}\frac{\gamma_j}{\beta_j} < \infty,$$

the quantity $\hat{e}_{n,d}^2(\boldsymbol{z})$ satisfies a $O(n^{-\frac{1}{2}})$ bound, with the implied constant independent of d.

It follows from a generalization of [36] that the optimal rate of convergence for QMC rules in weighted Sobolev spaces is $O(n^{-1+\delta})$ for any $\delta > 0$, with the implied constant independent of d, which leads to strong tractability. Further, there exist shifted rank-1 lattice rules that achieve this optimal rate of convergence when the weights satisfy

$$\sum_{j=1}^{\infty} \left(\frac{\gamma_j}{\beta_j}\right)^{\frac{1}{2(1-\delta)}} < \infty,$$

for any $\delta > 0$. By invoking the relationship between rank-1 lattice rules in weighted Korobov spaces and shifted rank-1 lattice rules in weighted Sobolev spaces, we can obtain analogous results for randomly shifted rank-1 lattice rules in weighted Sobolev spaces using results from the previous section, with the parameters α, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ replaced by 2, $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{\gamma}}$, where

$$\hat{\beta}_j = \beta_j + \frac{\gamma_j}{3} \quad \text{and} \quad \hat{\gamma}_j = \frac{\gamma_j}{2\pi^2}.$$

We give the results below in Theorem 9.4, Corollary 9.5, and Theorem 9.6. We thus conclude that the generating vector for randomly shifted rank-1 lattice rules constructed by Algorithm 6.4 achieves the optimal rate of convergence.

Theorem 9.4 [cf. Theorem 9.1] *Let n be a prime number and let $\frac{1}{2} < \lambda \leq 1$. Suppose there exists $\boldsymbol{z} \in \mathbb{Z}_n^d$ such that*

$$\hat{e}^2_{n,d}(\boldsymbol{z}) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d} \left(\left(\beta_j + \frac{\gamma_j}{3}\right)^{\lambda} + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(2\lambda) \right)^{\frac{1}{\lambda}}.$$

Then there exists $z_{d+1} \in \mathbb{Z}_n$ such that

$$\hat{e}^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{d+1} \left(\left(\beta_j + \frac{\gamma_j}{3}\right)^{\lambda} + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(2\lambda) \right)^{\frac{1}{\lambda}}.$$

Corollary 9.5 [cf. Corollary 9.2] *Let n be a prime number. We can construct $\boldsymbol{z} \in \mathbb{Z}_n^d$ component-by-component such that for all $s = 1, \ldots, d$,*

$$\hat{e}^2_{n,s}(z_1, \ldots, z_s) \leq 2^{\frac{1}{\lambda}} n^{-\frac{1}{\lambda}} \prod_{j=1}^{s} \left(\left(\beta_j + \frac{\gamma_j}{3}\right)^{\lambda} + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(2\lambda) \right)^{\frac{1}{\lambda}},$$

for all λ satisfying $\frac{1}{2} < \lambda \leq 1$. We can set $z_1 = 1$, and for s satisfying $2 \leq s \leq d$, each z_s can be found by minimizing $\hat{e}^2_{n,s}(z_1, \ldots, z_s)$ over the set $\mathbb{Z}_n$.

Theorem 9.6 [cf. Theorem 9.3] *Let n be a prime number and let $\boldsymbol{z}$ be constructed component-by-component as in Algorithm 6.4. Then this $\boldsymbol{z}$ satisfies*

$$\hat{e}_{n,d}(\boldsymbol{z}) \leq C_d(\delta)\, n^{-1+\delta} e_{0,d}, \quad \text{for all} \quad 0 < \delta \leq \tfrac{1}{2},$$

where

$$C_d(\delta) = 2^{1-\delta} \prod_{j=1}^{d} \left[1 + 2 \left(\frac{\frac{\gamma_j}{2\pi^2}}{\beta_j + \frac{\gamma_j}{3}} \right)^{\frac{1}{2(1-\delta)}} \zeta \left(\frac{1}{1-\delta} \right) \right]^{1-\delta},$$

and

$$e_{0,d} = \prod_{j=1}^{d} \left(\beta_j + \frac{\gamma_j}{3} \right)^{\frac{1}{2}}.$$

Moreover, if

$$\sum_{j=1}^{\infty} \left(\frac{\gamma_j}{\beta_j} \right)^{\frac{1}{2(1-\delta)}} < \infty,$$

then

$$C_d(\delta) \leq C_\infty(\delta) < \infty.$$

that is, $\hat{e}_{n,d}(\boldsymbol{z})$ *is* $O(n^{-1+\delta})$ *for* $\delta > 0$*, independently of* d*, with the* ε*-exponent of strong tractability (in a probabilistic sense) being* 1.

Chapter 10

Numerical Experiments on the Component-by-component Constructions

In this chapter, we outline some of the numerical experiments that were carried out on the construction of lattice rules in weighted Korobov and Sobolev spaces. Instead of including the results from each and every construction, we present here collective results for comparison purposes.

We consider weighted Korobov spaces with $\alpha = 2$ and $\boldsymbol{\beta} = \mathbf{1}$, and weighted Sobolev spaces with $\boldsymbol{a} = \mathbf{1}$ and $\boldsymbol{\beta} = \mathbf{1}$. For both function spaces, we consider different sequences of $\boldsymbol{\gamma}$ of two forms:

$$\gamma_j = r^j,\ 0 < r < 1, \quad \text{or} \quad \gamma_j = \frac{1}{j^r},\ r \geq 1.$$

To guarantee that the lattice rules constructed achieve strong tractability error bounds, we need the weights to satisfy (see Theorems 2.9 and 2.15):

$$\sum_{j=1}^{\infty} \gamma_j < \infty,$$

and for the optimal rate of convergence $O(n^{-1+\delta})$, $\delta > 0$, to be achieved, we require a more restrictive condition (see Theorems 9.3 and 9.6):

$$\sum_{j=1}^{\infty} \gamma_j^{\frac{1}{2(1-\delta)}} < \infty.$$

For example, the choice of $\gamma_j = 1/j$ fails both of these two conditions.

10.1 Experiments on the construction of shifted rank-1 lattice rules

We recall from Chapter 4 that a component-by-component algorithm, Algorithm 4.8, can be used to construct the generating vector and the shift of a shifted rank-1 lattice rule that achieves strong tractability error bounds in weighted Sobolev spaces. Here we present the worst-case errors from searches based on different choices of weights, and further discuss the behavior of these worst-case errors and their apparent relationships with the weights.

For weighted Sobolev spaces with $\boldsymbol{a} = \mathbf{1}$ and $\boldsymbol{\beta} = \mathbf{1}$, we consider four sequences of $\boldsymbol{\gamma}$:

$$\gamma_j = 0.5^j, \quad \gamma_j = 0.75^j, \quad \gamma_j = 0.9^j, \quad \text{and} \quad \gamma_j = \frac{1}{j^2}.$$

Some preliminary numerical searches for the generator vector and the shift up to 40 dimensions were carried out using Algorithm 4.8 with n taking the prime values 1009, 2003, and 4001. We present the values of the worst-case error $e_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta})$ and the root QMC mean $\sqrt{E_{n,d}}$ (see Lemma 2.17) in Tables 10.1 to 10.4 in steps of 10 dimensions.

The striking feature of the numerical results is that in all cases the worst-case errors $e_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta})$ for the computed rules are considerably smaller than the root QMC mean $\sqrt{E_{n,d}}$. It also seems, on comparing the results with $n = 1009$, 2003 and 4001, that the convergence of $e_{n,d}$ to zero as n increases is faster than the theoretically predicted $O(n^{-\frac{1}{2}})$.

Though the results are not presented here, some searches were also done for two other choices of γ_j, namely, $\gamma_j = 1/j$ and $\gamma_j = 1/j^{1.1}$. For the first choice, we expect tractability, but not strong tractability, whereas strong tractability is expected in the second case. The values of $e_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta})$ for the case $\gamma_j = 1/j^{1.1}$ and $d > 1$ were smaller than those in the case $\gamma_j = 1/j$, which in turn were smaller than those for the case $\gamma_j = 0.9^j$.

In practice, we do not know what the weights for a particular integrand

Table 10.1: Weighted Sobolev spaces with $\gamma_j = 0.5^j$

d	$e_{1009,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{1009,d}}$	$e_{2003,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{2003,d}}$	$e_{4001,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{4001,d}}$
10	5.8498e-04	1.4665e-02	3.1179e-04	1.0408e-02	1.6415e-04	7.3643e-03
20	5.8674e-04	1.4676e-02	3.1283e-04	1.0416e-02	1.6472e-04	7.3699e-03
30	5.8674e-04	1.4676e-02	3.1284e-04	1.0416e-02	1.6473e-04	7.3699e-03
40	5.8674e-04	1.4676e-02	3.1284e-04	1.0416e-02	1.6473e-04	7.3699e-03

Table 10.2: Weighted Sobolev spaces with $\gamma_j = 0.75^j$

d	$e_{1009,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{1009,d}}$	$e_{2003,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{2003,d}}$	$e_{4001,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{4001,d}}$
10	3.3418e-03	3.4271e-02	1.9454e-03	2.4324e-02	1.1048e-03	1.7210e-02
20	4.0446e-03	3.6585e-02	2.3876e-03	2.5966e-02	1.3733e-03	1.8372e-02
30	4.0938e-03	3.6719e-02	2.4188e-03	2.6061e-02	1.3915e-03	1.8440e-02
40	4.0968e-03	3.6726e-02	2.4207e-03	2.6067e-02	1.3926e-03	1.8443e-02

Table 10.3: Weighted Sobolev spaces with $\gamma_j = 0.9^j$

d	$e_{1009,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{1009,d}}$	$e_{2003,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{2003,d}}$	$e_{4001,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{4001,d}}$
10	1.5662e-02	8.2624e-02	9.5439e-03	5.8643e-02	5.6462e-03	4.1493e-02
20	4.5262e-02	1.4871e-01	2.8786e-02	1.0555e-01	1.7900e-02	7.4682e-02
30	6.3863e-02	1.8195e-01	4.0883e-02	1.2914e-01	2.5719e-02	9.1374e-02
40	7.1877e-02	1.9520e-01	4.6109e-02	1.3854e-01	2.9169e-02	9.8025e-02

Table 10.4: Weighted Sobolev spaces with $\gamma_j = 1/j^2$

d	$e_{1009,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{1009,d}}$	$e_{2003,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{2003,d}}$	$e_{4001,d}(\boldsymbol{z}, \boldsymbol{\Delta})$	$\sqrt{E_{4001,d}}$
10	8.6418e-04	1.8920e-02	4.6973e-04	1.3428e-02	2.4831e-04	9.5012e-03
20	9.7793e-04	1.9462e-02	5.3582e-04	1.3813e-02	2.8830e-04	9.7737e-03
30	1.0270e-03	1.9650e-02	5.6430e-04	1.3947e-02	3.0505e-04	9.8679e-03
40	1.0549e-03	1.9745e-02	5.8021e-04	1.4014e-02	3.1447e-04	9.9157e-03

will be. So one may ask the question of whether the shifted lattice rules found using Algorithm 4.8 for a particular choice of the sequence γ will be good for other choices of γ. As a numerical experiment, we took $n = 1009$ and used the values of z and Δ constructed above (which are for a particular choice of γ) for d up to 40 dimensions to calculate the values of $e_{n,d}(z, \Delta)$ for all the other three choices of γ. A summary of the results is given in Table 10.5.

Table 10.5: Maximum ratios of $e_{1009,d}$

	$\gamma_j = 1/j^2$	$\gamma_j = 0.5^j$	$\gamma_j = 0.75^j$	$\gamma_j = 0.9^j$
Rules found with $\gamma_j = 1/j^2$	1	1.003	1.061	1.131
Rules found with $\gamma_j = 0.5^j$	1.135	1	1.092	1.500
Rules found with $\gamma_j = 0.75^j$	1.036	1.013	1	1.037
Rules found with $\gamma_j = 0.9^j$	1.083	1.024	1.028	1

To describe what the numerical entries mean, consider the column headed $\gamma_j = 1/j^2$. Then each entry in the column is

$$\max_{1 \le d \le 40} \frac{e'_{1009,d}(z, \Delta)}{e_{1009,d}(z, \Delta)},$$

where both $e'_{1009,d}(z, \Delta)$ and $e_{1009,d}(z, \Delta)$ are calculated with $\gamma_j = 1/j^2$. However, $e'_{1009,d}(z, \Delta)$ is calculated by using the rule found by applying Algorithm 4.8 and taking the γ_j given in the corresponding row whereas $e_{1009,d}(z, \Delta)$ is calculated using the rule found by applying Algorithm 4.8 and taking $\gamma_j = 1/j^2$. Thus for example, in the column with $\gamma_j = 1/j^2$, we see an entry of 1.083 in the row with $\gamma_j = 0.9^j$. This entry of 1.083 means for each value of d, all the values of $e'_{1009,d}(z, \Delta)$ calculated with $\gamma_j = 1/j^2$ using the rules found by applying Algorithm 4.8 with $\gamma_j = 0.9^j$ were at most 8.3% larger than the corresponding values of $e_{1009,d}(z, \Delta)$. The numerical entries in the other three columns have a similar meaning.

10.2 Experiments on the construction of lattice rules with a composite number of points

For weighted Korobov spaces, we have developed in Chapter 3 an algorithm, Algorithm 3.10, for constructing rank-1 lattice rules. Similarly for weighted Sobolev spaces, we have Algorithm 4.8 in Chapter 4 for constructing shifted rank-1 lattice rules. For the latter algorithm, we have included, in the previous section, the results from some numerical experiments.

Both these algorithms were developed under the assumption that n was a prime number. But we knew from Chapter 5 that this does not have to be the case. Algorithms 5.10 and 5.15 allow the construction of rules with a composite number of points. What we are interested here is the answer to the question: how do the worse-case errors for rules with a composite number of points compare with those with a prime number of points?

For weighted Korobov spaces with $\alpha = 2$ and $\boldsymbol{\beta} = \mathbf{1}$, and weighted Sobolev spaces with $\boldsymbol{a} = \mathbf{1}$ and $\boldsymbol{\beta} = \mathbf{1}$, we consider three different sequences of $\boldsymbol{\gamma}$:

$$\gamma_j = \frac{1}{j^2}, \quad \gamma_j = 0.5^j, \quad \text{and} \quad \gamma_j = 0.9^j.$$

We carried out some numerical searches for the generating vector $\boldsymbol{z}$ of rank-1 lattice rules in weighted Korobov spaces using Algorithm 5.10, with n taking the values from 1004 to 1014 and from 1998 to 2008. Similarly in weighted Sobolev spaces, some numerical searches for the generating vector $\boldsymbol{z}$ and the shift $\boldsymbol{\Delta}$ of shifted rank-1 lattice rules were carried out using Algorithm 5.15. The worst-case errors for different values of n when $d = 40$ are presented in Tables 10.6 to 10.9. The entry c in each table is the number of distinct prime factors for the corresponding value of n.

Table 10.6: $e_{n,40}(\boldsymbol{z})$ in weighted Korobov spaces with n close to the prime 1009

n	c	$\gamma_j = 1/j^2$	$\gamma_j = 0.5^j$	$\gamma_j = 0.9^j$
1004	2	7.2061e-02	2.8876e-02	3.2624e+02
1005	3	7.2261e-02	2.8486e-02	3.2344e+02
1006	2	7.2412e-02	2.8697e-02	3.2569e+02
1007	2	7.1979e-02	2.8273e-02	3.2658e+02
1008	3	7.2872e-02	2.8857e-02	3.2473e+02
1009	1	7.1916e-02	2.8401e-02	3.2397e+02
1010	3	7.2743e-02	2.8696e-02	3.2363e+02
1011	2	7.2159e-02	2.8365e-02	3.2434e+02
1012	3	7.2969e-02	2.8873e-02	3.2421e+02
1013	1	7.2031e-02	2.8262e-02	3.2266e+02
1014	3	7.3358e-02	2.8549e-02	3.2461e+02

Table 10.7: $e_{n,40}(\boldsymbol{z})$ in weighted Korobov spaces with n close to the prime 2003

n	c	$\gamma_j = 1/j^2$	$\gamma_j = 0.5^j$	$\gamma_j = 0.9^j$
1998	3	4.6606e-02	1.7576e-02	2.3065e+02
1999	1	4.5766e-02	1.6921e-02	2.3075e+02
2000	2	4.6235e-02	1.6978e-02	2.3090e+02
2001	3	4.6139e-02	1.7420e-02	2.3052e+02
2002	4	4.6505e-02	1.7525e-02	2.3057e+02
2003	1	4.5647e-02	1.7013e-02	2.2993e+02
2004	3	4.6435e-02	1.7290e-02	2.2983e+02
2005	2	4.5903e-02	1.7030e-02	2.3034e+02
2006	3	4.6011e-02	1.7475e-02	2.2945e+02
2007	2	4.5952e-02	1.6822e-02	2.3057e+02
2008	2	4.5426e-02	1.7041e-02	2.3022e+02

Table 10.8: $e_{n,40}(\boldsymbol{z}, \boldsymbol{\Delta})$ in weighted Sobolev spaces with n close to the prime 1009

n	c	$\gamma_j = 1/j^2$	$\gamma_j = 0.5^j$	$\gamma_j = 0.9^j$
1004	2	1.0568e-03	5.8639e-04	7.3730e-02
1005	3	1.0874e-03	5.9505e-04	7.2327e-02
1006	2	1.0691e-03	6.0501e-04	7.2668e-02
1007	2	1.0665e-03	5.9117e-04	7.2635e-02
1008	3	1.0711e-03	5.9026e-04	7.2910e-02
1009	1	1.0549e-03	5.8674e-04	7.1877e-02
1010	3	1.0718e-03	6.0248e-04	7.2307e-02
1011	2	1.0414e-03	5.8636e-04	7.2378e-02
1012	3	1.0658e-03	5.9807e-04	7.3480e-02
1013	1	1.0541e-03	5.8458e-04	7.1902e-02
1014	3	1.0631e-03	5.9520e-04	7.2269e-02

Table 10.9: $e_{n,40}(\boldsymbol{z}, \boldsymbol{\Delta})$ in weighted Sobolev spaces with n close to the prime 2003

n	c	$\gamma_j = 1/j^2$	$\gamma_j = 0.5^j$	$\gamma_j = 0.9^j$
1998	3	6.0219e-04	3.2436e-04	4.6718e-02
1999	1	5.7508e-04	3.1156e-04	4.5740e-02
2000	2	5.8802e-04	3.1734e-04	4.6397e-02
2001	3	5.8377e-04	3.1967e-04	4.6751e-02
2002	4	5.9211e-04	3.1530e-04	4.6706e-02
2003	1	5.8021e-04	3.1284e-04	4.6109e-02
2004	3	5.8714e-04	3.1169e-04	4.7132e-02
2005	2	5.7738e-04	3.1274e-04	4.5700e-02
2006	3	5.8806e-04	3.1620e-04	4.7011e-02
2007	2	5.7742e-04	3.1353e-04	4.5943e-02
2008	2	5.8717e-04	3.1247e-04	4.6740e-02

We see from our results that in general, the higher the number of distinct prime factors, the larger the worst-case error, although the differences are not at all significant. The observed dependency of the worst-case error on c, the number of distinct prime factors of n, is not surprising as our theoretical bound also depends on c (see Corollaries 5.9 and 5.14). It is also worth mentioning that, though the results are not presented here, in all cases the worst-case errors are smaller than the root QMC mean in the corresponding spaces.

10.3 Experiments on the construction of intermediate-rank lattice rules

Recall that intermediate-rank lattice rules can be considered as rules formed by copying the first few dimensions of the points from rank-1 lattice rules. The motivation for such copying is that the first few variables in weighted spaces are in a sense more important than the rest as the weights were assumed to be non-increasing. Algorithms were developed in Chapter 7 for constructing these rules. Here we want to see if intermediate-rank lattice rules are better than rank-1 lattice rules with roughly the same number of points. More precisely, when $\ell = 2$, we want to know how many dimensions to copy, (that is, which value of $r = 1, 2,$ or 3 to take), to get better rules than rank-1 lattice rules.

For weighted Korobov spaces with $\alpha = 2$, $\boldsymbol{\beta} = \mathbf{1}$, and two choices of $\boldsymbol{\gamma}$:

$$\gamma_j = 0.9^j \quad \text{and} \quad \gamma_j = \frac{1}{j^2},$$

we construct the generating vector for intermediate-rank lattice rules up to 100 dimensions using Algorithm 7.9. We compare the worst-case errors for rules with different values of $r = 1, 2,$ and 3, and have a total number of points $N = \ell^r n$ being roughly 4000, 16000, and 64000. The results are presented in Tables 10.10 to 10.15 in steps of 10 dimensions. Each second column contains the worst-case error for rank-1 rules while the other three columns contain the worst-case error for r going from $r = 1$ to $r = 3$.

Table 10.10: $e_{N,d}$ in weighted Korobov spaces with N close to 4000, $\gamma_j = 0.9^j$

d	4001	$2003 \times 2^1 = 4006$	$1999 \times 2^1 = 3998$	$1009 \times 2^2 = 4036$	$997 \times 2^2 = 3988$	$503 \times 2^3 = 4024$	$499 \times 2^3 = 3992$
10	2.9726e+00	2.8068e+00	2.8005e+00	2.6666e+00	2.6874e+00	2.5965e+00	2.6068e+00
20	3.8737e+01	3.6466e+01	3.6455e+01	3.4687e+01	3.4922e+01	3.3752e+01	3.3887e+01
30	1.1022e+02	1.0374e+02	1.0372e+02	9.8675e+01	9.9337e+01	9.6009e+01	9.6392e+01
40	1.6309e+02	1.5348e+02	1.5346e+02	1.4598e+02	1.4696e+02	1.4204e+02	1.4260e+02
50	1.8768e+02	1.7661e+02	1.7659e+02	1.6798e+02	1.6911e+02	1.6344e+02	1.6409e+02
60	1.9719e+02	1.8556e+02	1.8554e+02	1.7650e+02	1.7768e+02	1.7172e+02	1.7241e+02
70	2.0063e+02	1.8879e+02	1.8878e+02	1.7957e+02	1.8077e+02	1.7472e+02	1.7542e+02
80	2.0185e+02	1.8994e+02	1.8992e+02	1.8066e+02	1.8187e+02	1.7578e+02	1.7648e+02
90	2.0227e+02	1.9034e+02	1.9032e+02	1.8104e+02	1.8225e+02	1.7615e+02	1.7685e+02
100	2.0242e+02	1.9048e+02	1.9046e+02	1.8118e+02	1.8239e+02	1.7628e+02	1.7698e+02

Table 10.11: $e_{N,d}$ in weighted Korobov spaces with N close to 16000, $\gamma_j = 0.9^j$

d	16007	$8009 \times 2^1 = 16018$	$7993 \times 2^1 = 15986$	$4003 \times 2^2 = 16012$	$4001 \times 2^2 = 16004$	$2003 \times 2^3 = 16024$	$1999 \times 2^3 = 15992$
10	1.4365e+00	1.3566e+00	1.3606e+00	1.2982e+00	1.2973e+00	1.2623e+00	1.2621e+00
20	1.9268e+01	1.8198e+01	1.8231e+01	1.7400e+01	1.7413e+01	1.6905e+01	1.6922e+01
30	5.4841e+01	5.1793e+01	5.1887e+01	4.9516e+01	4.9554e+01	4.8109e+01	4.8157e+01
40	8.1141e+01	7.6628e+01	7.6767e+01	7.3258e+01	7.3314e+01	7.1176e+01	7.1247e+01
50	9.3371e+01	8.8176e+01	8.8337e+01	8.4298e+01	8.4363e+01	8.1902e+01	8.1984e+01
60	9.8103e+01	9.2645e+01	9.2813e+01	8.8570e+01	8.8638e+01	8.6053e+01	8.6138e+01
70	9.9815e+01	9.4261e+01	9.4433e+01	9.0115e+01	9.0184e+01	8.7554e+01	8.7641e+01
80	1.0042e+02	9.4832e+01	9.5004e+01	9.0661e+01	9.0730e+01	8.8084e+01	8.8172e+01
90	1.0063e+02	9.5032e+01	9.5205e+01	9.0852e+01	9.0922e+01	8.8270e+01	8.8358e+01
100	1.0070e+02	9.5102e+01	9.5275e+01	9.0919e+01	9.0988e+01	8.8335e+01	8.8423e+01

Table 10.12: $e_{N,d}$ in weighted Korobov spaces with N close to 64000, $\gamma_j = 0.9^j$

d	64007	$32009 \times 2^1 = 64018$	$32003 \times 2^1 = 64006$	$16007 \times 2^2 = 64028$	$16001 \times 2^2 = 64004$	$8009 \times 2^3 = 64072$	$7993 \times 2^3 = 63944$
10	6.8423e-01	6.4784e-01	6.4773e-01	6.1683e-01	6.1797e-01	5.9937e-01	6.0015e-01
20	9.6190e+00	9.1124e+00	9.0949e+00	8.6927e+00	8.6945e+00	8.4445e+00	8.4523e+00
30	2.7406e+01	2.5958e+01	2.5908e+01	2.4763e+01	2.4768e+01	2.4055e+01	2.4077e+01
40	4.0552e+01	3.8408e+01	3.8336e+01	3.6640e+01	3.6647e+01	3.5592e+01	3.5625e+01
50	4.6664e+01	4.4197e+01	4.4114e+01	4.2162e+01	4.2170e+01	4.0956e+01	4.0995e+01
60	4.9029e+01	4.6436e+01	4.6350e+01	4.4299e+01	4.4307e+01	4.3032e+01	4.3072e+01
70	4.9885e+01	4.7247e+01	4.7159e+01	4.5072e+01	4.5080e+01	4.3783e+01	4.3824e+01
80	5.0187e+01	4.7533e+01	4.7444e+01	4.5345e+01	4.5353e+01	4.4048e+01	4.4089e+01
90	5.0293e+01	4.7633e+01	4.7544e+01	4.5441e+01	4.5449e+01	4.4141e+01	4.4182e+01
100	5.0330e+01	4.7668e+01	4.7579e+01	4.5474e+01	4.5483e+01	4.4173e+01	4.4215e+01

Table 10.13: $e_{N,d}$ in weighted Korobov spaces with N close to 4000, $\gamma_j = 1/j^2$

d	4001	$2003 \times 2^1 = 4006$	$1999 \times 2^1 = 3998$	$1009 \times 2^2 = 4036$	$997 \times 2^2 = 3988$	$503 \times 2^3 = 4024$	$499 \times 2^3 = 3992$
10	1.9338e-02	1.8362e-02	1.8036e-02	2.0006e-02	2.0218e-02	2.5298e-02	2.5381e-02
20	2.5421e-02	2.3923e-02	2.3776e-02	2.6554e-02	2.6843e-02	3.3678e-02	3.3951e-02
30	2.7770e-02	2.6094e-02	2.6001e-02	2.9126e-02	2.9474e-02	3.7124e-02	3.7290e-02
40	2.9017e-02	2.7262e-02	2.7181e-02	3.0495e-02	3.0864e-02	3.8956e-02	3.9126e-02
50	2.9795e-02	2.7989e-02	2.7913e-02	3.1362e-02	3.1728e-02	4.0095e-02	4.0269e-02
60	3.0326e-02	2.8489e-02	2.8415e-02	3.1954e-02	3.2320e-02	4.0875e-02	4.1051e-02
70	3.0714e-02	2.8853e-02	2.8780e-02	3.2384e-02	3.2751e-02	4.1444e-02	4.1620e-02
80	3.1008e-02	2.9130e-02	2.9058e-02	3.2711e-02	3.3079e-02	4.1875e-02	4.2052e-02
90	3.1240e-02	2.9348e-02	2.9276e-02	3.2970e-02	3.3337e-02	4.2213e-02	4.2390e-02
100	3.1426e-02	2.9523e-02	2.9453e-02	3.3178e-02	3.3545e-02	4.2485e-02	4.2662e-02

Table 10.14: $e_{N,d}$ in weighted Korobov spaces with N close to 16000, $\gamma_j = 1/j^2$

d	16007	$8009 \times 2^1 = 16018$	$7993 \times 2^1 = 15986$	$4003 \times 2^2 = 16012$	$4001 \times 2^2 = 16004$	$2003 \times 2^3 = 16024$	$1999 \times 2^3 = 15992$
10	7.0679e-03	6.6226e-03	6.7551e-03	7.4726e-03	7.4423e-03	9.2985e-03	9.3671e-03
20	9.7139e-03	9.1387e-03	9.2672e-03	1.0362e-02	1.0344e-02	1.2975e-02	1.3059e-02
30	1.0786e-02	1.0146e-02	1.0266e-02	1.1513e-02	1.1516e-02	1.4491e-02	1.4543e-02
40	1.1364e-02	1.0691e-02	1.0808e-02	1.2139e-02	1.2150e-02	1.5307e-02	1.5349e-02
50	1.1727e-02	1.1033e-02	1.1145e-02	1.2528e-02	1.2543e-02	1.5818e-02	1.5854e-02
60	1.1977e-02	1.1268e-02	1.1378e-02	1.2796e-02	1.2814e-02	1.6168e-02	1.6204e-02
70	1.2159e-02	1.1438e-02	1.1547e-02	1.2993e-02	1.3012e-02	1.6425e-02	1.6461e-02
80	1.2299e-02	1.1567e-02	1.1676e-02	1.3143e-02	1.3163e-02	1.6622e-02	1.6657e-02
90	1.2409e-02	1.1670e-02	1.1778e-02	1.3261e-02	1.3282e-02	1.6778e-02	1.6812e-02
100	1.2498e-02	1.1753e-02	1.1861e-02	1.3357e-02	1.3379e-02	1.6904e-02	1.6938e-02

Table 10.15: $e_{N,d}$ in weighted Korobov spaces with N close to 64000, $\gamma_j = 1/j^2$

d	64007	32009×2^1 $= 64018$	32003×2^1 $= 64006$	16007×2^2 $= 64028$	16001×2^2 $= 64004$	8009×2^3 $= 64072$	7993×2^3 $= 63944$
10	2.5983e-03	2.4131e-03	2.4454e-03	2.6945e-03	2.6743e-03	3.3548e-03	3.3135e-03
20	3.7412e-03	3.5099e-03	3.5290e-03	3.9372e-03	3.9465e-03	4.9385e-03	4.9097e-03
30	4.2141e-03	3.9582e-03	3.9767e-03	4.4501e-03	4.4667e-03	5.5924e-03	5.5795e-03
40	4.4705e-03	4.2019e-03	4.2200e-03	4.7333e-03	4.7496e-03	5.9532e-03	5.9446e-03
50	4.6325e-03	4.3564e-03	4.3735e-03	4.9111e-03	4.9270e-03	6.1803e-03	6.1750e-03
60	4.7448e-03	4.4624e-03	4.4798e-03	5.0334e-03	5.0484e-03	6.3377e-03	6.3334e-03
70	4.8270e-03	4.5399e-03	4.5573e-03	5.1227e-03	5.1371e-03	6.4533e-03	6.4493e-03
80	4.8901e-03	4.5991e-03	4.6166e-03	5.1912e-03	5.2052e-03	6.5416e-03	6.5378e-03
90	4.9398e-03	4.6460e-03	4.6635e-03	5.2452e-03	5.2593e-03	6.6113e-03	6.6077e-03
100	4.9801e-03	4.6840e-03	4.7014e-03	5.2890e-03	5.3032e-03	6.6678e-03	6.6645e-03

We can see from the results that for $\gamma_j = 0.9^j$, copying is good in at least the first three dimensions, but for $\gamma_j = 1/j^2$, it is only good to copy in the first dimension. This seems reasonable as in the first few dimensions the sequence $\{0.9, 0.81, 0.729, \ldots\}$ decays slower than $\{1, 1/4, 1/9, \ldots\}$, and so in the former case, the third variable is still fairly important while this is not the situation in the latter case.

The phenomenon is also supported by our earlier analysis. Theorem 7.5 and Lemma 7.6 together suggest that it would be advantageous to copy in the first r dimensions if $\ell = 2$, $\alpha = 2$ and

$$\frac{\gamma_r}{\beta_r} > \frac{6}{\pi^2} \approx 0.6079.$$

For $\gamma_j = 0.9^j$, this is obviously satisfied when $r = 1$, $r = 2$, and $r = 3$. For $\gamma_j = 1/j^2$, this is only satisfied when $r = 1$. Because Lemma 7.6 provides only a sufficient condition for $\rho_{2,r}$ to be less than one, a direct calculation of $\rho_{2,r}$ was done and it showed that $\rho_{2,r}$ was greater than one when $r = 2$ and $r = 3$.

10.4 Experiments on the construction of randomly shifted rank-1 lattice rules when $n = pq$

The total cost for the construction of an n-point shifted rank-1 lattice rule up to d dimensions using Algorithm 4.8 is roughly $O(n^3 d^2)$ operations. This can be reduced to $O(n^3 d)$ operations if the implementation stores the products at the expense of $O(n^2)$ storage. But even then, it would take a horrendous amount of time and vast memory storage to construct rules with up to a few thousand points. Our numerical experiments went as far as 4001 points up to only 40 dimensions, and the computation time required using 650MHz PCs at the time was approximately three weeks.

Since then Algorithm 6.4 was developed which left out the construction of the shift, that is, we generate a number of shifts randomly once the generating vector was constructed. The cost of the construction was reduced to $O(n^2 d)$ operations at the expense of only $O(n)$ storage. This allowed us to construct rules as far as having 64007 points up to 360 dimensions.

In Chapter 8, we considered rules with the number of points being a product of two distinct primes. We developed Algorithm 8.7 which guarantees the square worst-case error to be bounded by the QMC mean, and when the two primes are roughly the same, the cost of the construction is only $O(n^{1.5}d)$ operations with $O(n)$ storage requirement. We have also proposed an even cheaper but not yet theoretically justified algorithm, Algorithm 8.9, which only requires $O(nd)$ operations at the expense of $O(n)$ storage. The numerical experiments here are aimed at finding out whether or not Algorithm 8.7 performs as well as Algorithm 6.4, and how Algorithm 8.9 performs.

For weighted Sobolev spaces with $\boldsymbol{a} = \mathbf{1}$, $\boldsymbol{\beta} = \mathbf{1}$ and two sequences of $\boldsymbol{\gamma}$:

$$\gamma_j = 0.9^j \quad \text{and} \quad \gamma_j = 1/j^2,$$

we first consider these values of $n = pq$ with p and q being consecutive prime numbers:

$$2021 = 43 \times 47, \quad 8633 = 89 \times 97, \quad \text{and} \quad 32399 = 179 \times 181.$$

For each n, we compare the worst-case errors for the 100-dimensional rules constructed by

1. Full search (using Algorithm 6.4)
2. Partial search with $p < q$ (using Algorithm 8.7)
3. Partial search with $p > q$ (using Algorithm 8.7)
4. Separate search (using Algorithm 8.9)

We also compare the four values above with the root QMC mean $\sqrt{E_{n,d}}$. The results of these comparisons are given in Tables 10.16 to 10.21 in steps of 10 dimensions.

Table 10.16: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 2021 = 43\times47$, $\gamma_j = 0.9^j$

d	Full	Partial 43	Partial 47	Separate	$\sqrt{E_{n,d}}$
10	1.0030e-02	1.0714e-02	1.0611e-02	1.8537e-02	5.8381e-02
20	2.9740e-02	3.1235e-02	3.1139e-02	4.6375e-02	1.0508e-01
30	4.2048e-02	4.3879e-02	4.3877e-02	6.1188e-02	1.2857e-01
40	4.7351e-02	4.9240e-02	4.9264e-02	6.7611e-02	1.3792e-01
50	4.9365e-02	5.1290e-02	5.1310e-02	7.0125e-02	1.4134e-01
60	5.0099e-02	5.2034e-02	5.2053e-02	7.0895e-02	1.4256e-01
70	5.0360e-02	5.2297e-02	5.2317e-02	7.1180e-02	1.4298e-01
80	5.0452e-02	5.2391e-02	5.2411e-02	7.1280e-02	1.4313e-01
90	5.0485e-02	5.2424e-02	5.2443e-02	7.1320e-02	1.4318e-01
100	5.0496e-02	5.2435e-02	5.2455e-02	7.1336e-02	1.4320e-01

Table 10.17: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 8633 = 89\times97$, $\gamma_j = 0.9^j$

d	Full	Partial 89	Partial 97	Separate	$\sqrt{E_{n,d}}$
10	3.2940e-03	3.6384e-03	3.6468e-03	6.3585e-03	2.8247e-02
20	1.0741e-02	1.1617e-02	1.1594e-02	1.5587e-02	5.0841e-02
30	1.5626e-02	1.6684e-02	1.6644e-02	2.1750e-02	6.2205e-02
40	1.7812e-02	1.8878e-02	1.8870e-02	2.4162e-02	6.6733e-02
50	1.8653e-02	1.9713e-02	1.9720e-02	2.5630e-02	6.8388e-02
60	1.8959e-02	2.0019e-02	2.0023e-02	2.5961e-02	6.8975e-02
70	1.9068e-02	2.0129e-02	2.0130e-02	2.6099e-02	6.9181e-02
80	1.9106e-02	2.0168e-02	2.0169e-02	2.6144e-02	6.9253e-02
90	1.9120e-02	2.0181e-02	2.0183e-02	2.6158e-02	6.9278e-02
100	1.9124e-02	2.0186e-02	2.0187e-02	2.6164e-02	6.9286e-02

Table 10.18: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 32399 = 179 \times 181$, $\gamma_j = 0.9^j$

d	Full	Partial 179	Partial 181	Separate	$\sqrt{E_{n,d}}$
10	1.2274e-03	1.3711e-03	1.3266e-03	2.2289e-03	1.4581e-02
20	4.3265e-03	4.6855e-03	4.5624e-03	6.7407e-03	2.6244e-02
30	6.4592e-03	6.8705e-03	6.8194e-03	1.0121e-02	3.2110e-02
40	7.4199e-03	7.8676e-03	7.7940e-03	1.1357e-02	3.4447e-02
50	7.7870e-03	8.2427e-03	8.1711e-03	1.1991e-02	3.5302e-02
60	7.9214e-03	8.3808e-03	8.3094e-03	1.2174e-02	3.5605e-02
70	7.9692e-03	8.4295e-03	8.3585e-03	1.2232e-02	3.5711e-02
80	7.9861e-03	8.4468e-03	8.3762e-03	1.2252e-02	3.5748e-02
90	7.9921e-03	8.4529e-03	8.3823e-03	1.2259e-02	3.5761e-02
100	7.9942e-03	8.4551e-03	8.3845e-03	1.2262e-02	3.5765e-02

Table 10.19: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 2021 = 43 \times 47$, $\gamma_j = 1/j^2$

d	Full	Partial 43	Partial 47	Separate	$\sqrt{E_{n,d}}$
10	5.4217e-04	5.7233e-04	5.7138e-04	1.6506e-03	1.3368e-02
20	6.0878e-04	6.4959e-04	6.4970e-04	1.9882e-03	1.3752e-02
30	6.3779e-04	6.8141e-04	6.8122e-04	2.1203e-03	1.3884e-02
40	6.5414e-04	6.9933e-04	6.9871e-04	2.1708e-03	1.3952e-02
50	6.6506e-04	7.1220e-04	7.1075e-04	2.2005e-03	1.3992e-02
60	6.7280e-04	7.2132e-04	7.1958e-04	2.2232e-03	1.4019e-02
70	6.7872e-04	7.2820e-04	7.2602e-04	2.2310e-03	1.4039e-02
80	6.8339e-04	7.3403e-04	7.3127e-04	2.2398e-03	1.4054e-02
90	6.8722e-04	7.3878e-04	7.3543e-04	2.2478e-03	1.4065e-02
100	6.9041e-04	7.4273e-04	7.3900e-04	2.2508e-03	1.4074e-02

Table 10.20: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 8633 = 89 \times 97$, $\gamma_j = 1/j^2$

d	Full	Partial 89	Partial 97	Separate	$\sqrt{E_{n,d}}$
10	1.4341e-04	1.5792e-04	1.5703e-04	5.2701e-04	6.4682e-03
20	1.6550e-04	1.8207e-04	1.8080e-04	6.5811e-04	6.6537e-03
30	1.7508e-04	1.9207e-04	1.8969e-04	6.6919e-04	6.7178e-03
40	1.8048e-04	1.9761e-04	1.9560e-04	6.9607e-04	6.7503e-03
50	1.8398e-04	2.0126e-04	1.9944e-04	7.0316e-04	6.7700e-03
60	1.8647e-04	2.0371e-04	2.0225e-04	7.0484e-04	6.7832e-03
70	1.8835e-04	2.0562e-04	2.0437e-04	7.0767e-04	6.7926e-03
80	1.8980e-04	2.0714e-04	2.0604e-04	7.1477e-04	6.7997e-03
90	1.9098e-04	2.0837e-04	2.0738e-04	7.1614e-04	6.8052e-03
100	1.9196e-04	2.0941e-04	2.0846e-04	7.1889e-04	6.8097e-03

Table 10.21: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 32399 = 179 \times 181$, $\gamma_j = 1/j^2$

d	Full	Partial 179	Partial 181	Separate	$\sqrt{E_{n,d}}$
10	4.3053e-05	4.7329e-05	4.7885e-05	2.0938e-04	3.3389e-03
20	5.0979e-05	5.5936e-05	5.6405e-05	2.1974e-04	3.4346e-03
30	5.4281e-05	5.9338e-05	5.9815e-05	2.2552e-04	3.4677e-03
40	5.6173e-05	6.1318e-05	6.1781e-05	2.2757e-04	3.4845e-03
50	5.7383e-05	6.2608e-05	6.2973e-05	2.3266e-04	3.4947e-03
60	5.8254e-05	6.3560e-05	6.3847e-05	2.3407e-04	3.5015e-03
70	5.8912e-05	6.4266e-05	6.4505e-05	2.3502e-04	3.5063e-03
80	5.9426e-05	6.4816e-05	6.5017e-05	2.3575e-04	3.5100e-03
90	5.9840e-05	6.5230e-05	6.5446e-05	2.3695e-04	3.5128e-03
100	6.0179e-05	6.5599e-05	6.5794e-05	2.3735e-04	3.5151e-03

We see that the results for the two partial searches are very similar, and they are both only slightly worse than the results for the full search. The results for the separate search are much worse than those of the full or partial searches, but all the results indicate that they are better than the root QMC mean. This is certainly encouraging, and perhaps we could give the theoretical justification of this algorithm in the future.

Finally, we take advantage of the decomposition $n = pq$ and construct rules with much larger values of n:

$$2005007 = 1409 \times 1423,\ 4003997 = 1999 \times 2003,\ \text{and}\ 8037211 = 2833 \times 2837.$$

We construct 100-dimensional rules by partial search and separate search (items 2 and 4 from before), that is, using Algorithms 8.7 and 8.9. The results are presented in Tables 10.22 to 10.24. We see once again that the results from the separate searches are not as good as those of the partial searches, but better than the root QMC mean.

Table 10.22: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 2005007 = 1409 \times 1423$

	$\gamma_j = 0.9^j$			$\gamma_j = 1/j^2$		
d	Partial	Separate	$\sqrt{E_{n,d}}$	Partial	Separate	$\sqrt{E_{n,d}}$
10	5.7794e-05	1.9373e-04	1.8535e-03	1.1521e-06	2.9195e-05	4.2443e-04
20	2.6699e-04	5.1684e-04	3.3361e-03	1.4982e-06	2.9509e-05	4.3660e-04
30	4.3114e-04	8.1808e-04	4.0818e-03	1.6530e-06	2.9629e-05	4.4081e-04
40	5.0699e-04	9.1275e-04	4.3789e-03	1.7393e-06	2.9696e-05	4.4294e-04
50	5.3671e-04	9.5625e-04	4.4875e-03	1.7970e-06	2.9737e-05	4.4423e-04
60	5.4740e-04	9.6980e-04	4.5260e-03	1.8364e-06	2.9765e-05	4.4510e-04
70	5.5132e-04	9.7482e-04	4.5395e-03	1.8659e-06	2.9786e-05	4.4572e-04
80	5.5265e-04	9.7639e-04	4.5442e-03	1.8896e-06	2.9820e-05	4.4618e-04
90	5.5314e-04	9.7696e-04	4.5459e-03	1.9068e-06	2.9837e-05	4.4655e-04
100	5.5331e-04	9.7733e-04	4.5464e-03	1.9218e-06	2.9850e-05	4.4684e-04

Table 10.23: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 4003997 = 1999 \times 2003$

	$\gamma_j = 0.9^j$			$\gamma_j = 1/j^2$		
d	Partial	Separate	$\sqrt{E_{n,d}}$	Partial	Separate	$\sqrt{E_{n,d}}$
10	3.3113e-05	5.8331e-05	1.3116e-03	6.2568e-07	1.9506e-06	3.0034e-04
20	1.6371e-04	2.8567e-04	2.3608e-03	8.2383e-07	2.8095e-06	3.0895e-04
30	2.6707e-04	4.5837e-04	2.8884e-03	9.1087e-07	2.9218e-06	3.1193e-04
40	3.1648e-04	5.2667e-04	3.0987e-03	9.6121e-07	3.0128e-06	3.1344e-04
50	3.3621e-04	5.5585e-04	3.1755e-03	9.9372e-07	3.3042e-06	3.1436e-04
60	3.4341e-04	5.6852e-04	3.2028e-03	1.0178e-06	3.3429e-06	3.1497e-04
70	3.4595e-04	5.7233e-04	3.2123e-03	1.0359e-06	3.3982e-06	3.1541e-04
80	3.4682e-04	5.7342e-04	3.2157e-03	1.0497e-06	3.4205e-06	3.1574e-04
90	3.4712e-04	5.7386e-04	3.2168e-03	1.0604e-06	3.4752e-06	3.1599e-04
100	3.4723e-04	5.7402e-04	3.2172e-03	1.0697e-06	3.4869e-06	3.1620e-04

Table 10.24: $\hat{e}_{n,d}$ in weighted Sobolev spaces with $n = 8037211 = 2833 \times 2837$

	$\gamma_j = 0.9^j$			$\gamma_j = 1/j^2$		
d	Partial	Separate	$\sqrt{E_{n,d}}$	Partial	Separate	$\sqrt{E_{n,d}}$
10	1.9339e-05	5.1847e-05	9.2577e-04	3.3957e-07	9.6089e-07	2.1199e-04
20	1.0078e-04	2.1839e-04	1.6663e-03	4.4923e-07	1.1555e-06	2.1807e-04
30	1.6721e-04	3.0910e-04	2.0387e-03	5.0124e-07	1.3196e-06	2.2017e-04
40	1.9870e-04	3.5657e-04	2.1871e-03	5.2935e-07	1.3727e-06	2.2124e-04
50	2.1133e-04	3.7280e-04	2.2413e-03	5.4968e-07	1.4227e-06	2.2188e-04
60	2.1590e-04	3.7976e-04	2.2606e-03	5.6308e-07	1.6201e-06	2.2231e-04
70	2.1751e-04	3.8261e-04	2.2673e-03	5.7390e-07	1.6361e-06	2.2262e-04
80	2.1809e-04	3.8343e-04	2.2697e-03	5.8239e-07	1.6573e-06	2.2285e-04
90	2.1829e-04	3.8373e-04	2.2705e-03	5.8914e-07	1.6676e-06	2.2303e-04
100	2.1836e-04	3.8386e-04	2.2708e-03	5.9461e-07	1.6751e-06	2.2318e-04

10.5 Experiments on the observed rate of convergence

In Chapter 9, we have shown that for n prime, the rank-1 lattice rules constructed by Algorithms 3.10, and the randomly shifted rank-1 lattice rules constructed by Algorithms 6.4 achieve the optimal rate of convergence in weighted Korobov and Sobolev spaces respectively. Our goal for the numerical experiments here is to determine whether the optimal rate of convergence is observed as the theory suggested.

For weighted Sobolev spaces with $\boldsymbol{a} = \mathbf{1}$ and $\boldsymbol{\beta} = \mathbf{1}$, we consider six sequences of $\boldsymbol{\gamma}$:

$$\gamma_j = 0.9^j, \quad \gamma_j = 0.5^j, \quad \gamma_j = 0.1^j, \quad \gamma_j = \frac{1}{j^2}, \quad \gamma_j = \frac{1}{j^6}, \quad \text{and} \quad \gamma_j = \frac{1}{j}.$$

Note that the last sequence does not satisfy

$$\sum_{j=1}^{\infty} \gamma_j^{\frac{1}{2(1-\delta)}} < \infty,$$

for any $\delta > 0$, which is the required condition in the theory, for the optimal rate of convergence $O(n^{-1+\delta})$ to be achieved. We search for the generating vector $\boldsymbol{z}$ for randomly shifted rank-1 lattice rules using Algorithm 6.4, with d up to 100 and n taking the prime values 4001, 8009, 16001, 32003, and 64007. We want to see if the numerical results from the component-by-component search actually show the optimal rate of convergence, that is, we are interested in the value of ω in

$$\hat{e}_{n,d}(\boldsymbol{z}) = O(n^{-\omega}),$$

which can be estimated by the ratio

$$\widetilde{\omega} := \frac{\log\left(\frac{\hat{e}_{n_1,d}(\boldsymbol{z}_1)}{\hat{e}_{n_2,d}(\boldsymbol{z}_2)}\right)}{\log\left(\frac{n_2}{n_1}\right)}. \tag{10.1}$$

Let $B_{n,d}(\delta)$ denote the upper bound for $\hat{e}_{n,d}(\boldsymbol{z})$ given in Theorem 9.6. Then

$$\hat{e}_{n,d}(\boldsymbol{z}) \le B_{n,d}(\delta) = C_d(\delta) n^{-1+\delta} e_{0,d}, \qquad \text{for all } 0 < \delta \le 0.5,$$

where

$$e_{0,d} = \prod_{j=1}^{d} \left(1 + \frac{\gamma_j}{3}\right)^{\frac{1}{2}}$$

and

$$C_d(\delta) = 2^{1-\delta} \prod_{j=1}^{d} \left[1 + 2 \left(\frac{\frac{\gamma_j}{2\pi^2}}{1 + \frac{\gamma_j}{3}} \right)^{\frac{1}{2(1-\delta)}} \zeta\left(\frac{1}{1-\delta}\right) \right]^{1-\delta}$$

We present in Tables 10.25 to 10.30 the values of $\hat{e}_{n,100}(\boldsymbol{z})$, $B_{n,100}(\delta^*)$, and ω^* for various values of n. Here δ^* denotes the value of δ that minimizes $B_{n,d}(\delta)$ and $\omega^* = 1 - \delta^*$. We also present the values of $\widetilde{\omega}$ given in (10.1) from the successive values of $\hat{e}_{n,100}(\boldsymbol{z})$.

Table 10.25: Weighted Sobolev spaces with $\gamma_j = 0.9^j$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	3.2010e-02	0.66603	1.6990e-01	0.500
8009	2.0162e-02	0.65442	1.1997e-01	0.505
16001	1.2819e-02	0.66611	8.4361e-02	0.513
32003	8.0782e-03	0.66968	5.8963e-02	0.521
64007	5.0783e-03		4.1000e-02	0.528

Table 10.26: Weighted Sobolev spaces with $\gamma_j = 0.5^j$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	1.9597e-04	0.91456	1.0723e-02	0.725
8009	1.0388e-04	0.92081	6.4617e-03	0.735
16001	5.4924e-05	0.93704	3.8741e-03	0.744
32003	2.8686e-05	0.95460	2.3070e-03	0.752
64007	1.4801e-05		1.3664e-03	0.759

Table 10.27: Weighted Sobolev spaces with $\gamma_j = 0.1^j$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	3.4726e-05		2.6450e-03	0.871
8009	1.7383e-05	0.99704	1.4421e-03	0.877
16001	8.7079e-06	0.99884	7.8445e-04	0.883
32003	4.3599e-06	0.99799	4.2474e-04	0.888
64007	2.1834e-06	0.99771	2.2922e-04	0.892

Table 10.28: Weighted Sobolev spaces with $\gamma_j = 1/j^2$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	3.7846e-04		1.6971e-02	0.663
8009	2.0432e-04	0.88819	1.0682e-02	0.671
16001	1.1011e-04	0.89329	6.6941e-03	0.679
32003	6.0764e-05	0.85760	4.1700e-03	0.686
64007	3.2954e-05	0.88275	2.5849e-03	0.693

Table 10.29: Weighted Sobolev spaces with $\gamma_j = 1/j^6$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	1.0653e-04		5.3547e-03	0.833
8009	5.3407e-05	0.99493	2.9944e-03	0.842
16001	2.6763e-05	0.99829	1.6675e-03	0.850
32003	1.3425e-05	0.99533	9.2295e-04	0.857
64007	6.7205e-06	0.99822	5.0849e-04	0.863

Table 10.30: Weighted Sobolev spaces with $\gamma_j = 1/j$

n	$\hat{e}_{n,100}(\boldsymbol{z})$	$\widetilde{\omega}$	$B_{n,100}(\delta^*)$	ω^*
4001	9.2597e-03		7.3429e-02	0.524
		0.69545		
8009	5.7146e-03		5.0892e-02	0.532
		0.67798		
16001	3.5744e-03		3.5132e-02	0.539
		0.68976		
32003	2.2159e-03		2.4125e-02	0.546
		0.67894		
64007	1.3841e-03		1.6493e-02	0.552

We see from the numerical results that the values of the apparent rate of convergence $\widetilde{\omega}$ are close to 1 when $\gamma_j = 0.1^j$ and $\gamma_j = 1/j^6$, while in other cases values close to 1 cannot be seen with our choices of n. It would appear that the apparent rate of convergence depends on the rate of decay of the weights γ: the faster the rate of decay, the closer the value of $\widetilde{\omega}$ to 1. The theoretical bounds, even for the optimal choice of δ^*, are generally far from sharp. This is mainly due to the large value of $\zeta(\frac{1}{1-\delta})$ for δ close to 0. A different approach to the analysis might yield sharper bounds.

Chapter 11

Constructing Sobol' Sequences in High Dimensions that Satisfy Sobol's Property A

An algorithm to generate Sobol' sequences to approximate integrals in up to 40 dimensions has been previously given by Bratley and Fox in Algorithm 659 [4]. Here we provide more primitive polynomials and 'direction numbers' so as to allow the generation of Sobol' sequences to approximate integrals in up to 1111 dimensions. The direction numbers given generate Sobol' sequences that satisfy Sobol's so-called Property A.

11.1 Sobol' sequences

One technique for approximating the d-dimensional integral is to make use of Sobol' sequences. These were proposed by Sobol' in [37] and a computer implementation in Fortran 77 was subsequently given by Bratley and Fox in Algorithm 659 (see [4] for details). Other implementations are available as C, Fortran 77, or Fortran 90 routines in the popular Numerical Recipes collection of software (for example, see [28]). However, as given, all these implementations have a fairly heavy restriction on the maximum value of d allowed. For

Algorithm 659, Sobol' sequences may be generated to approximate integrals in up to 40 dimensions, while the Numerical Recipes routines allow the generation of Sobol' sequences to approximate integrals in up to six dimensions only.

As new methods become available for these integrals, one might wish to compare these new methods with Sobol' sequences. Thus it would be desirable to extend these existing implementations such as Algorithm 659 so they may be used for higher-dimensional integrals. We remark that Sobol' sequences are now considered to be examples of (t,d)-sequences in base 2. The general theory of these low discrepancy (t,d)-sequences in base b is discussed in detail in Chapter 4 of Niederreiter's book [23].

11.1.1 Sobol' sequence generator

The generation of Sobol' sequences is clearly explained in [4]. We review the main points so as to show what extra data would be required to allow Algorithm 659 to generate Sobol' sequences to approximate integrals in more than 40 dimensions. To generate the j-th component of the points in a Sobol' sequence, we need to choose a primitive polynomial of some degree s_j in the field $\mathbb{Z}_2$, that is, a polynomial of the form

$$x^{s_j} + a_{1,j}x^{s_j-1} + \cdots + a_{s_j-1,j}x + 1,$$

where the coefficients $a_{1,j}, \ldots, a_{s_j-1,j}$ are either 0 or 1.

We use these coefficients to define a sequence $\{m_{1,j}, m_{2,j}, \ldots\}$ of positive integers by the recurrence relation

$$\begin{aligned} m_{k,j} &= 2a_{1,j}m_{k-1,j} \oplus 2^2 a_{2,j}m_{k-2,j} \oplus \cdots \oplus 2^{s_j-1}a_{s_j-1,j}m_{k-s_j+1,j} \\ &\qquad \oplus 2^{s_j} m_{k-s_j,j} \oplus m_{k-s_j,j}, \end{aligned} \tag{11.1}$$

for $k \geq s_j+1$, where $\oplus$ is the bit-by-bit exclusive-or operator. The initial values $m_{1,j}, m_{2,j}, \ldots, m_{s_j,j}$ can be chosen freely provided that each $m_{k,j}$, $1 \leq k \leq s_j$, is odd and less than 2^k. The 'direction numbers' $\{v_{1,j}, v_{2,j}, \ldots\}$ are defined by

$$v_{k,j} := \frac{m_{k,j}}{2^k}.$$

Then $x_{i,j}$, the j-th component of the i-th point in a Sobol' sequence is given by

$$x_{i,j} = b_1 v_{1,j} \oplus b_2 v_{2,j} \oplus \cdots ,$$

where b_ℓ is the ℓ-th bit from the right when i is written in binary, that is, $(\ldots b_2 b_1)_2$ is the binary representation of i. In practice, a more efficient Gray code implementation proposed by Antonov and Saleev is used; see [2] or [4] for details.

We then see that the implementation in [4] may be used to generate Sobol' sequences to approximate integrals in more than 40 dimensions by providing more data in the form of primitive polynomials and direction numbers (or equivalently, values of $m_{1,j}, m_{2,j}, \ldots, m_{s_j,j}$). When generating such Sobol' sequences, we need to ensure that the primitive polynomials used to generate each component are different and that the initial values of the $m_{k,j}$'s are chosen differently for any two primitive polynomials of the same degree. The error bounds for Sobol' sequences given in [37] indicate we should use primitive polynomials of as low a degree as possible.

11.1.2 Sobol's property A

We will discuss how additional primitive polynomials may be obtained in the next section. After these primitive polynomials have been found, we need to decide upon the initial values of the $m_{k,j}$ for $1 \leq k \leq s_j$. As explained above, all we require is that they be odd and that $m_{k,j} < 2^k$. Thus we could just choose them randomly subject to these two constraints. However, Sobol' in [38] introduced an extra uniformity condition known as Property A. Geometrically, if the cube $[0,1]^d$ is divided up by the planes $x_j = 1/2$ into 2^d equally-sized subcubes, then a sequence of points belonging to $[0,1]^d$ possesses Property A if, after dividing the sequence into consecutive blocks of 2^d points, each one of the points in any block belongs to a different subcube.

Property A is not that useful to have for large d because of the computational time required to approximate an integral using 2^d points. Also, Property A is not enough to ensure that there are no bad correlations between pairs of dimensions (see Section 7 of [22] for a discussion). Nevertheless, Property A is still a reasonable criterion to use in deciding upon a choice of the initial $m_{k,j}$. In [38], Sobol' showed that a Sobol' sequence used to approximate a d-dimensional integral possesses Property A if and only if

$$\det(V_d) = 1 \pmod 2,$$

where V_d is the $d \times d$ binary matrix defined by

$$V_d := \begin{bmatrix} v_{1,1,1} & v_{2,1,1} & & v_{d,1,1} \\ v_{1,2,1} & v_{2,2,1} & & v_{d,2,1} \\ & & & \vdots \\ v_{1,d,1} & v_{2,d,1} & & v_{d,d,1} \end{bmatrix}, \qquad (11.2)$$

with $v_{k,j,1}$ denoting the first bit after the binary point of $v_{k,j}$.

The primitive polynomials and direction numbers used in Algorithm 659 are taken from [39] and a subset of this data may be found in [38]. Though it is mentioned in [38] that Property A is satisfied for $d \leq 16$, that is, $\det(V_d) = 1 \pmod 2$ for all $d \leq 16$, our calculations showed that Property A is actually satisfied for $d \leq 20$. As a result, we change the values of the $m_{k,j}$ for $21 \leq j \leq 40$, but keep the primitive polynomials. For $j \geq 41$ we obtain additional primitive polynomials.

The number of primitive polynomials of degree s is $\phi(2^s - 1)/s$, where ϕ is Euler's totient function. Including the special case for $j = 1$ when all the $m_{k,1}$ are 1, this allows us to approximate integrals in up to dimension $d = 1111$ if we use all the primitive polynomials of degree 13 or less.

We then choose values of the $m_{k,j}$ so that we can generate Sobol' sequences satisfying Property A in dimensions d up to 1111. This is done by generating some values randomly, but these are subsequently modified so that the condition $\det(V_d) = 1 \pmod 2$ is satisfied for all d up to 1111. This process involves evaluating values of the $v_{k,j,1}$'s to obtain the matrix V_d and then evaluating the determinant of V_d. A more detailed discussion of this strategy is given in the next section. It is not difficult to produce values to generate Sobol' points for approximating integrals in even higher dimensions.

11.2 Generating the primitive polynomials and direction numbers

In this section, we describe in detail the steps we use to find the extra data required for the generation of Sobol' sequences up to 1111 dimensions.

11.2.1 Obtaining primitive polynomials

Recall that we are interested in the primitive polynomials of the form

$$x^{s_j} + a_{1,j}x^{s_j-1} + \cdots + a_{s_j-1,j}x + 1,$$

where the coefficients $a_{1,j}, \ldots, a_{s_j-1,j}$ are either 0 or 1. We will represent such a polynomial by $P_{s_j,a_j}(x)$, where a_j is the decimal value of the binary number $(a_{1,j}a_{2,j}\ldots a_{s_j-1,j})_2$, that is,

$$a_j = \sum_{k=1}^{s_j-1} a_{k,j}2^{s_j-k-1}.$$

Note that though this representation of the primitive polynomial using a_j is also used in [4], the Fortran 77 routines associated with [4] use $\bar{a}_j$ instead, where $\bar{a}_j$ is the decimal value of the binary number $(1a_{1,j}a_{2,j}\ldots a_{s_j-1,j}1)_2$. Thus

$$\bar{a}_j = 2^{s_j} + 2a_j + 1.$$

Finding out whether a given polynomial in $\mathbb{Z}_2$ is a primitive polynomial is not a trivial task. Fortunately, there are computer programs available on the

Internet that will compute all the possible primitive polynomials of specified degree. We obtain the coefficients using a computer program downloaded from

ftp://helsbreth.org/pub/helsbret/random/lfsr_s.c.

In order to check that the primitive polynomials generated from this program were correct, they were compared with those generated by using a different computer program which we downloaded from

http://www.theory.csc.uvic.ca/~cos/dis/distribute.pl.cgi?package=poly.c.

For $d \leq 40$, we keep the primitive polynomials as they are in Algorithm 659. For $d \geq 41$, we adopt a systematic approach in which we arrange the primitive polynomials of the same degree in increasing order of the a_j. In Algorithm 659 all the primitive polynomials up to degree 7 were used plus three out of the 16 primitive polynomials of degree 8. The remaining 13 are used for dimensions $d = 41$ to $d = 53$. The 48 primitive polynomials of degree 9 are used in the same way for d from 54 to 101, There are 60 primitive polynomials of degree 10 that are used for $102 \leq d \leq 161$, 176 of degree 11 used for $162 \leq d \leq 337$, 144 of degree 12 used for $338 \leq d \leq 481$, and 630 polynomials of degree 13 used for d from 482 to 1111.

11.2.2 Evaluation of the $v_{k,j,1}$

In order to test for Property A, we need to form the matrix V_d (see (11.2)) which contains entries consisting of the first bit after the binary point of the direction numbers. Thus we do not need to evaluate the directions numbers fully, but only need the first bit of each direction number. Since the initial direction numbers $v_{k,j}$ are given by $m_{k,j}/2^k$, for $1 \leq k \leq s_j$, then it is clear that $v_{k,j,1} = 1$ if $m_{k,j}/2^k \geq 1/2$ and $v_{k,j,1} = 0$ if $m_{k,j}/2^k < 1/2$. Such considerations lead to the following lemma.

Lemma 11.1 *For $j = 1$, assume we have the special case in which all the $m_{k,1}$ have the value 1. Then*

$$v_{1,1,1} = 1 \quad \text{and} \quad v_{k,1,1} = 0 \text{ for } k \geq 2.$$

Given choices of primitive polynomials and initial values $m_{k,j}$ for $1 \le k \le s_j$, then

$$v_{k,j,1} = \begin{cases} 0, & \text{if } m_{k,j} < 2^{k-1}, \\ 1, & \text{if } m_{k,j} \ge 2^{k-1}, \end{cases} \qquad 1 \le k \le s_j, \quad j \ge 2.$$

To form V_d, we also need values of the $v_{k,j,1}$ for $k > s_j$. The required result is given in the next lemma.

Lemma 11.2 *For $j \ge 2$ and $k > s_j$, we have*

$$v_{k,j,1} = a_{1,j}v_{k-1,j,1} \oplus a_{2,j}v_{k-2,j,1} \oplus \cdots \oplus a_{s_j-1,j}v_{k-s_j+1,j,1} \oplus v_{k-s_j,j,1}.$$

Proof. Because $v_{k,j} = m_{k,j}/2^k$, it follows from the recurrence relation (11.1) that

$$v_{k,j} = a_{1,j}v_{k-1,j} \oplus a_{2,j}v_{k-2,j} \oplus \cdots \oplus a_{s_j-1,j}v_{k-s_j+1,j} \oplus v_{k-s_j,j} \oplus \frac{v_{k-s_j,j}}{2^{s_j}}.$$

Since $\oplus$ is a bit-by-bit operator and $v_{k-s_j,j}/2^{s_j} < 1/2$, the required result follows. □

11.2.3 Finding initial values of the $m_{k,j}$

Recall that for $j \le 20$, we use the existing $m_{k,j}$ in Algorithm 659 as Property A is already satisfied. For j between 21 and 40, we start with the existing $m_{k,j}$ in Algorithm 659 and for j successively taking the values 41 . . . 1111, we randomly generate $m_{1,j}, \ldots, m_{s_j,j}$ such that they are odd and satisfy $m_{k,j} < 2^k$. We can then use Lemmas 11.1 and 11.2 to form V_j for each j from 21 to 1111 and test whether $\det(V_j) = 1 \pmod 2$ is satisfied. If it is, we can then proceed to the next value of j.

If the determinant is $0 \pmod 2$, then we need to modify the initial values of $m_{k,j}$'s so that $\det(V_j) = 1 \pmod 2$ is satisfied. Since $v_{k,j,1}$ is 0 when $m_{k,j} \in [1, 2^{k-1})$ and 1 when $m_{k,j} \in [2^{k-1}, 2^k)$, then $v_{k,j,1}$ may be changed by replacing $m_{k,j}$ by $(m_{k,j} + 2^{k-1}) \pmod{2^k}$.

Starting with $m_{2,j}$, we replace it by $(m_{2,j} + 2) \pmod 4$ (which in effect changes the value of $v_{2,j,1}$) and then re-evaluate the determinant. If the determinant is still $0 \pmod 2$, we change this new value of $m_{2,j}$ back to its original value and then replace $m_{3,j}$ by $(m_{3,j} + 4) \pmod 8$ and re-evaluate the determinant. We repeat the same process for $m_{4,j}, m_{5,j}, \ldots$ until the determinant is $1 \pmod 2$ or until $m_{s_j,j}$ is reached. If this latter stage is reached, then we generate another random set of $m_{1,j}, \ldots, m_{s_j,j}$ and repeat the process. As it turned out in our calculations, this was never the case.

11.2.4 Evaluation of the determinant

The evaluation of the determinant can be simplified since when working in $\mathbb{Z}_2$:

i. Swapping rows does not change the determinant.

ii. Adding a row to another (and likewise subtracting a row from another) is equivalent to applying an exclusive-or operation. This also leaves the determinant unchanged.

Because bit operations like the exclusive-or operation are very quick in a programming language such as C++, the determinant of V_d may be found quite quickly by attempting to row-reduce V_d to an upper triangular matrix with 1's all the way down its main diagonal. If we succeed, the determinant is 1. If at some stage we end up with a row of zeros, then the determinant is 0.

This process may be speeded up by making use of the fact that once we have the $m_{k,j}$ for $1 \leq k \leq s_j$ and $1 \leq j \leq d$, then V_d is fixed and so are the first d rows of V_j for $j > d$. We first row-reduce the first 20 rows of V_{1111} so that we have 1's down the main diagonal and 0's below the 1's. (This is possible because the determinants of $V_1, \ldots, V_{20}$ are all 1.) Then to evaluate the determinant of V_j for each j from 21 to 1111, we only need to row-reduce one extra row each time and thus avoid the repetitions in row operations.

11.3 Results of calculations

A table containing values of j, s_j, a_j, $\bar{a}_j$, and $m_{k,j}$, $k = 1, \ldots, s_j$, for j going from 2 to 1111 is available as an ascii text file which may be downloaded from

http://www.math.waikato.ac.nz/˜stephenj/soboltab.txt.

We present here these values up to 100 dimensions. In the case $j = 1$, we follow the Bratley and Fox implementation and use the special case of $m_{k,1} = 1$ for $k \geq 1$. The values of $m_{k,j}$ given in brackets are those obtained by the recurrence relation (11.1).

j	s_j	a_j	$\bar{a}_j$	$m_{1,j}$	$m_{2,j}$	$m_{3,j}$	$m_{4,j}$	$m_{5,j}$	$m_{6,j}$	$m_{7,j}$	$m_{8,j}$	$m_{9,j}$	$m_{10,j}$	$m_{11,j}$	$m_{12,j}$	$m_{13,j}$	
1				1	1	1	1	1	1	1	1	1	1	1	1	1	···
2	1	0	3	1	(3)	(5)	(15)	(17)	(51)	(85)	(255)	(257)	(771)	(1285)	(3855)	(4369)	
3	2	1	7	1	1	(7)	(11)	(13)	(61)	(67)	(79)	(465)	(721)	(823)	(4091)	(4125)	
4	3	1	11	1	3	7	(5)	(7)	(43)	(49)	(147)	(439)	(1013)	(727)	(987)	(5889)	
5	3	2	13	1	1	5	(3)	(15)	(51)	(125)	(141)	(177)	(759)	(267)	(1839)	(6929)	
6	4	1	19	1	3	1	1	(9)	(59)	(25)	(89)	(321)	(835)	(833)	(4033)	(3913)	
7	4	4	25	1	1	3	7	(31)	(47)	(109)	(173)	(181)	(949)	(471)	(2515)	(6211)	
8	5	2	37	1	3	3	9	9	(57)	(43)	(43)	(225)	(113)	(1601)	(579)	(1731)	
9	5	13	59	1	3	7	13	3	(35)	(89)	(9)	(235)	(929)	(1341)	(3863)	(1347)	
10	5	7	47	1	1	5	11	27	(53)	(69)	(25)	(103)	(615)	(913)	(977)	(6197)	
11	5	14	61	1	3	5	1	15	(19)	(113)	(115)	(411)	(157)	(1725)	(3463)	(2817)	
12	5	11	55	1	1	7	3	29	(51)	(47)	(97)	(233)	(39)	(2021)	(2909)	(5459)	
13	5	4	41	1	3	7	7	21	(61)	(55)	(19)	(59)	(761)	(1905)	(3379)	(8119)	
14	6	1	67	1	1	1	9	23	37	(97)	(97)	(353)	(169)	(375)	(1349)	(5121)	
15	6	16	97	1	3	3	5	19	33	(3)	(197)	(329)	(983)	(893)	(3739)	(7669)	
16	6	13	91	1	1	3	13	11	7	(37)	(101)	(463)	(657)	(1599)	(347)	(2481)	
17	6	22	109	1	1	7	13	25	5	(83)	(255)	(385)	(647)	(415)	(387)	(7101)	
18	6	19	103	1	3	5	11	7	11	(103)	(29)	(111)	(581)	(605)	(2881)	(2677)	
19	6	25	115	1	1	1	3	13	39	(27)	(203)	(475)	(505)	(819)	(2821)	(1405)	
20	7	1	131	1	3	1	15	17	63	13	(65)	(451)	(833)	(975)	(1873)	(7423)	
21	7	32	193	1	1	5	5	1	59	33	(195)	(263)	(139)	(915)	(1959)	(4853)	
22	7	4	137	1	3	3	3	25	17	115	(177)	(19)	(147)	(1715)	(1929)	(2465)	
23	7	8	145	1	1	7	15	29	15	41	(105)	(249)	(719)	(1223)	(2389)	(4599)	
24	7	7	143	1	3	1	7	3	23	79	(17)	(275)	(81)	(1367)	(3251)	(2887)	
25	7	56	241	1	3	7	9	31	29	17	(47)	(369)	(337)	(663)	(1149)	(1715)	···

j	s_j	a_j	$\bar{a}_j$	$m_{1,j}$	$m_{2,j}$	$m_{3,j}$	$m_{4,j}$	$m_{5,j}$	$m_{6,j}$	$m_{7,j}$	$m_{8,j}$	$m_{9,j}$	$m_{10,j}$	$m_{11,j}$	$m_{12,j}$	$m_{13,j}$	
26	7	14	157	1	1	5	13	11	3	29	(169)	(393)	(829)	(629)	(243)	(5595)	···
27	7	28	185	1	1	1	9	5	21	119	(109)	(421)	(989)	(1541)	(1545)	(5689)	
28	7	19	167	1	1	3	1	23	13	75	(149)	(333)	(375)	(469)	(1131)	(441)	
29	7	50	229	1	3	7	11	27	31	73	(143)	(217)	(873)	(989)	(3749)	(3137)	
30	7	21	171	1	1	7	7	19	25	105	(213)	(469)	(131)	(1667)	(143)	(4485)	
31	7	42	213	1	3	1	5	21	9	7	(7)	(357)	(211)	(571)	(1323)	(2215)	
32	7	31	191	1	1	1	15	5	49	59	(253)	(21)	(733)	(1251)	(3497)	(3557)	
33	7	62	253	1	3	1	1	1	33	65	(191)	(193)	(967)	(451)	(2499)	(483)	
34	7	37	203	1	3	5	15	17	19	21	(155)	(229)	(447)	(481)	(1571)	(3781)	
35	7	41	211	1	1	7	11	13	29	3	(175)	(247)	(177)	(721)	(983)	(3195)	
36	7	55	239	1	3	7	5	7	11	113	(63)	(297)	(57)	(483)	(4021)	(5213)	
37	7	59	247	1	1	5	11	15	19	61	(47)	(147)	(471)	(1201)	(3657)	(989)	
38	8	14	285	1	1	1	1	9	27	89	7	(497)	(465)	(1457)	(3217)	(185)	
39	8	56	369	1	1	3	7	31	15	45	23	(61)	(197)	(415)	(1163)	(7323)	
40	8	21	299	1	3	3	9	25	25	107	39	(361)	(763)	(1435)	(929)	(1697)	
41	8	22	301	1	1	7	7	3	63	21	217	(473)	(9)	(1775)	(1199)	(7467)	
42	8	38	333	1	3	5	7	5	55	71	141	(445)	(87)	(1105)	(891)	(5153)	
43	8	47	351	1	1	5	1	23	17	79	27	(173)	(93)	(1057)	(2021)	(5475)	
44	8	49	355	1	1	5	15	7	63	19	53	(53)	(973)	(1017)	(531)	(2315)	
45	8	50	357	1	1	3	15	3	49	71	181	(341)	(557)	(831)	(339)	(3927)	
46	8	52	361	1	3	3	15	17	19	61	169	(141)	(623)	(1567)	(1403)	(3893)	
47	8	67	391	1	3	3	13	23	41	41	35	(7)	(461)	(985)	(2943)	(7977)	
48	8	70	397	1	1	1	3	3	59	57	15	(319)	(991)	(287)	(2269)	(7449)	
49	8	84	425	1	3	1	3	3	3	121	207	(231)	(357)	(1491)	(189)	(4273)	
50	8	97	451	1	3	5	15	21	57	87	45	(391)	(569)	(235)	(3261)	(4931)	···

j	s_j	a_j	$\bar{a}_j$	$m_{1,j}$	$m_{2,j}$	$m_{3,j}$	$m_{4,j}$	$m_{5,j}$	$m_{6,j}$	$m_{7,j}$	$m_{8,j}$	$m_{9,j}$	$m_{10,j}$	$m_{11,j}$	$m_{12,j}$	$m_{13,j}$	
51	8	103	463	1	1	1	5	25	33	119	247	(339)	(667)	(411)	(1663)	(43)	...
52	8	115	487	1	1	1	9	25	49	55	185	(487)	(851)	(1843)	(1499)	(443)	
53	8	122	501	1	3	5	7	23	53	85	117	(295)	(161)	(995)	(365)	(6265)	
54	9	8	529	1	3	3	13	11	57	121	41	235	(865)	(291)	(2339)	(7981)	
55	9	13	539	1	1	3	3	19	57	119	81	307	(417)	(737)	(1443)	(739)	
56	9	16	545	1	3	3	7	3	39	11	223	495	(113)	(1715)	(3059)	(4343)	
57	9	22	557	1	3	3	5	11	21	23	151	417	(913)	(1843)	(4019)	(8021)	
58	9	25	563	1	3	1	11	31	7	61	81	57	(657)	(1075)	(2993)	(187)	
59	9	44	601	1	1	3	9	7	53	11	189	151	(249)	(137)	(3739)	(161)	
60	9	47	607	1	3	7	1	9	9	35	61	19	(761)	(779)	(3391)	(5929)	
61	9	52	617	1	1	5	9	5	55	33	95	119	(569)	(937)	(397)	(3313)	
62	9	55	623	1	3	7	1	17	15	43	185	375	(873)	(699)	(1135)	(4729)	
63	9	59	631	1	1	3	5	23	59	107	23	451	(137)	(745)	(2699)	(6685)	
64	9	62	637	1	1	7	7	17	19	113	73	55	(217)	(761)	(2383)	(5983)	
65	9	67	647	1	3	1	13	17	49	101	113	449	(69)	(1671)	(1685)	(2449)	
66	9	74	661	1	3	3	9	25	31	29	239	501	(797)	(1719)	(1367)	(6837)	
67	9	81	675	1	1	3	9	13	3	87	85	53	(613)	(1189)	(967)	(3789)	
68	9	82	677	1	1	5	1	11	39	119	9	185	(725)	(1813)	(1089)	(1605)	
69	9	87	687	1	1	1	7	31	5	97	201	317	(309)	(1445)	(901)	(3715)	
70	9	91	695	1	1	3	3	27	5	29	83	17	(253)	(437)	(3559)	(4647)	
71	9	94	701	1	3	5	5	19	41	17	53	21	(485)	(1063)	(3873)	(3497)	
72	9	103	719	1	1	5	1	17	9	89	183	487	(469)	(485)	(2473)	(2301)	
73	9	104	721	1	1	7	11	23	19	5	203	13	(997)	(1549)	(347)	(2167)	
74	9	109	731	1	3	7	11	7	9	127	91	347	(437)	(1623)	(1195)	(4447)	
75	9	122	757	1	1	7	13	5	57	89	149	393	(557)	(1213)	(2571)	(3873)	...

j	s_j	a_j	$\bar{a}_j$	$m_{1,j}$	$m_{2,j}$	$m_{3,j}$	$m_{4,j}$	$m_{5,j}$	$m_{6,j}$	$m_{7,j}$	$m_{8,j}$	$m_{9,j}$	$m_{10,j}$	$m_{11,j}$	$m_{12,j}$	$m_{13,j}$	
76	9	124	761	1	1	1	7	11	25	119	101	15	(285)	(1925)	(2301)	(2411)	...
77	9	137	787	1	1	1	7	19	1	117	13	391	(623)	(2047)	(1119)	(5145)	
78	9	138	789	1	3	3	9	19	15	103	111	307	(903)	(1133)	(3001)	(3867)	
79	9	143	799	1	3	3	9	7	51	105	239	189	(859)	(149)	(3145)	(5051)	
80	9	145	803	1	1	1	1	13	11	41	3	381	(331)	(775)	(1343)	(4783)	
81	9	152	817	1	3	1	1	21	19	83	205	71	(287)	(877)	(619)	(6919)	
82	9	157	827	1	3	5	3	21	61	25	253	163	(503)	(925)	(3471)	(7117)	
83	9	167	847	1	1	1	9	7	53	41	247	99	(79)	(359)	(1047)	(3999)	
84	9	173	859	1	3	5	15	9	29	55	121	467	(511)	(725)	(3991)	(1337)	
85	9	176	865	1	3	7	1	11	19	69	189	167	(87)	(1813)	(3781)	(5955)	
86	9	181	875	1	3	5	5	1	11	117	169	433	(59)	(301)	(2183)	(7555)	
87	9	182	877	1	1	1	13	5	9	49	179	337	(635)	(1983)	(3079)	(3083)	
88	9	185	883	1	3	7	1	21	21	127	197	257	(779)	(1133)	(3173)	(7971)	
89	9	191	895	1	3	5	9	11	19	29	175	179	(31)	(949)	(2535)	(6703)	
90	9	194	901	1	3	3	9	13	43	1	217	47	(187)	(841)	(1277)	(855)	
91	9	199	911	1	1	3	9	25	13	99	249	385	(39)	(1419)	(2889)	(5623)	
92	9	218	949	1	3	1	9	9	13	53	195	23	(83)	(137)	(3151)	(5923)	
93	9	220	953	1	3	5	9	7	41	83	95	117	(935)	(329)	(987)	(2283)	
94	9	227	967	1	1	7	13	7	25	15	63	369	(743)	(627)	(1141)	(1939)	
95	9	229	971	1	3	1	11	27	31	31	19	425	(39)	(1969)	(3191)	(3545)	
96	9	230	973	1	3	7	3	15	9	73	7	207	(651)	(593)	(817)	(3005)	
97	9	234	981	1	3	5	5	25	11	115	5	433	(847)	(1425)	(883)	(1535)	
98	9	236	985	1	1	1	11	15	19	35	75	301	(847)	(979)	(339)	(57)	
99	9	241	995	1	3	7	11	21	5	21	217	147	(955)	(929)	(1441)	(4645)	
100	9	244	1001	1	1	3	13	17	53	89	245	333	(407)	(611)	(3297)	(1131)	...

References

[1] Andrews, G. E. (1994). *Number Theory*, Dover, New York.

[2] Antonov, I. A. and Saleev, V. M. (1979). *An economic method of computing LP_τ-sequences*, Zh. vȳchisl. Mat. mat. Fiz., **19**, 243–245. English translation: U.S.S.R. Comput. Maths. Math. Phys., **19**, 252–256.

[3] Aronszajn, N. (1950). *Theory of reproducing kernels*, Trans. Amer. Math. Soc., **68**, 337–404.

[4] Bratley, P. and Fox, B. L. (1988). *Algorithm 659: Implementing Sobol's quasirandom sequence generator*, ACM Trans. Math. Softw., **14**, 88–100.

[5] Cranley, R. and Patterson, T. N. L. (1976). *Randomization of number theoretic methods for multiple integration*, SIAM J. Numer. Anal., **13**, 904–914.

[6] Disney, S. (1990). *Error bounds for rank 1 lattice quadrature rules modulo composites*, Monatsh. Math., **110**, 89–100.

[7] Hardy, G. H., Littlewood, J. E. and Pólya, G. (1934). *Inequalities*, Cambridge University Press, Cambridge.

[8] Hickernell, F. J. (1998). *A generalized discrepancy and quadrature error bound*, Math. Comp., **67**, 299–322.

[9] Hickernell, F. J. (1998). *Lattice rules: How well do they measure up?*, Random and Quasi-Random Point Sets (P. Hellekalek and G. Larcher, eds.), Lecture Notes in Statistics, vol. 138, Springer-Verlag, New York, 109–166.

[10] Hickernell, F. J. and Hong, H. S. (2002). *Quasi-Monte Carlo methods and their randomizations*, Proceedings of the IMS Workshop on Applied Probability, to appear.

[11] Hickernell, F. J. and Woźniakowski, H. (2000). *Integration and approximation in arbitrary dimensions*, Adv. Comput. Math., **12**, 25–58.

[12] Hickernell, F. J. and Woźniakowski, H. (2001). *Tractability of multivariate integration for periodic functions*, J. Complexity, **17**, 660–682.

[13] Hua, L. K. and Wang, Y. (1981). *Applications of number theory to numerical analysis*, Springer Verlag, Berlin; Science Press, Beijing.

[14] Joe, S. (1990). *Randomization of lattice rules for numerical multiple integration*, J. Comput. Appl. Math., **31**, 299–304.

[15] Joe, S. and Disney, S. A. R. (1993). *Intermediate rank lattice rules for multidimensional integration*, SIAM J. Numer. Anal., **30**, 569–582.

[16] Joe, S. and Kuo, F. Y. (2002). *Remark on Algorithm 659: Implementing Sobol's quasirandom sequence generator*, ACM Trans. Math. Softw., submitted.

[17] Joe, S. and Sloan, I. H. (1992). *Embedded lattice rules for multidimensional integration*, SIAM J. Numer. Anal., **29**, 1119–1135.

[18] Korobov, N. M. (1960). *Properties and calculation of optimal coefficients*, Doklady Akademii Nauk SSSR, **132**, 1009–10 (Russian). English translation: Soviet Mathematics Doklady, **1**, 696–700.

[19] Kuo, F. Y. (2002). *Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces*, J. Complexity, submitted.

[20] Kuo, F. Y. and Joe, S. (2002). *Component-by-component construction of good lattice rules with a composite number of points*, J. Complexity, to appear.

[21] Lindgren, B. W. (1976). *Statistical Theory* (3rd edn), Collier Macmillan, New York.

[22] Morokoff, W. J. and Caflisch R. E. (1992). *Quasi-random sequences and their discrepancies*, SIAM J. Sci. Comput., **15**, 1251–1279.

[23] Niederreiter, H. (1992). *Random number generation and quasi-Monte Carlo methods*, SIAM, Philadelphia.

[24] Novak, E., Sloan, I. H. and Woźniakowski, H. (1997). *Tractability of tensor product linear operators*, J. Complexity, **13**, 387–418.

[25] Novak, E. and Woźniakowski, H. (2001). *Intractability results for integration and discrepancy*, J. Complexity, **17**, 388–441.

[26] Owen, A. B. (1995). *Randomly permuted (t, m, s)-nets and (t, s)-sequences*, in Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (H. Niederreiter and P. J.-S Shiue, eds), Lecture Notes in Statistics 106, Springer-Verlag, New York, 299–317.

[27] Paskov, S. H. and Traub, J. F. (1995). *Faster valuation of financial derivatives*, J. Portfolio Management, **22**, 113–120.

[28] Press, W. H., Teukolsky, S. A., Vetterling, W. T. and Flannery, B. P. (1992). *Numerical recipes in Fortran 77: The art of scientific computing* (2nd edn), Cambridge University Press, Cambridge.

[29] Sloan, I. H. and Joe, S. (1994). *Lattice methods for multiple integration*, Clarendon Press, Oxford.

[30] Sloan, I. H., Kuo, F. Y. and Joe, S. (2002). *On the step-by-step construction of quasi-Monte Carlo integration rules that achieve strong tractability error bounds in weighted Sobolev spaces*, Math. Comp., to appear.

[31] Sloan, I. H., Kuo, F. Y. and Joe, S. (2002). *Constructing randomly shifted lattice rules in weighted Sobolev spaces*, SIAM J. Numer. Anal., to appear.

[32] Sloan, I. H. and Lyness, J. N. (1989). *The representation of lattice quadrature rules as multiple sums*, Math. Comp., **52**, 81–94.

[33] Sloan, I. H. and Reztsov, A. V. (2002). *Component-by-component construction of good lattice rules*, Math. Comp., **71**, 263–273.

[34] Sloan, I. H. and Woźniakowski, H. (1997). *An intractability result for multiple integration*, Math. Comp., **66**, 1119–1124.

[35] Sloan, I. H. and Woźniakowski, H. (1998). *When are quasi-Monte Carlo algorithms efficient for high dimensional integrals?*, J. Complexity, **14**, 1–33.

[36] Sloan, I. H. and Woźniakowski, H. (2001). *Tractability of multivariate integration for weighted Korobov classes*, J. Complexity, **17**, 697–721.

[37] Sobol', I. M. (1967). *On the distribution of points in a cube and the approximate evaluation of integrals*, Zh. vȳchisl. Mat. mat. Fiz., **7**, 784–802. English translation: U.S.S.R. Comput. Maths. Math. Phys., **7**, 86–112.

[38] Sobol', I. M. (1976). *Uniformly distributed sequences with an additional uniform property*, Zh. vȳchisl. Mat. mat. Fiz., **16**, 1332–1337. English translation: U.S.S.R. Comput. Maths. Math. Phys., **16**, 236–242.

[39] Sobol', I. M. and Levitan, Y. L. (1976). *The production of points uniformly distributed in a multidimensional cube*, Preprint 40, Institute of Applied Mathematics, USSR Academy of Sciences. (In Russian)

[40] Woźniakowski, H. (1994). *Tractability and strong tractability of linear multivariate problems*, J. Complexity, **10**, 96–128.

[41] Woźniakowski, H. (1994). *Tractability and strong tractability of multivariate tensor product problems*, Proceedings 2nd Gauss Symposium, München, 1993, J. Comput. Inform., **4**, 1–19.