New developments in the construction of lattice rules

Applications of lattice rules to high-dimensional integration problems from mathematical finance

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Benjamin James Waterhouse

UNSW
THE UNIVERSITY OF NEW SOUTH WALES
SYDNEY • AUSTRALIA

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Abstract

There are many problems in mathematical finance which require the evaluation of a multivariate integral. Since these problems typically involve the discretisation of a continuous random variable, the dimension of the integrand can be in the thousands, tens of thousands or even more.

For such problems the Monte Carlo method has been a powerful and popular technique. This is largely related to the fact that the performance of the method is independent of the number of dimensions. Traditional quasi-Monte Carlo techniques are typically not independent of the dimension and as such have not been suitable for high-dimensional problems. However, recent work has developed new types of quasi-Monte Carlo point sets which can be used in practically limitless dimension. Among these types of point sets are Sobol′ sequences, Faure sequences, Niederreiter-Xing sequences, digital nets and lattice rules. In this thesis, we will concentrate on results concerning lattice rules.

The typical setting for analysis of these new quasi-Monte Carlo point sets is the worst-case error in a weighted function space. There has been much work on constructing point sets with small worst-case errors in the weighted Korobov and Sobolev spaces. However, many of the integrands which arise in the area of mathematical finance do not lie in either of these spaces. One common problem is that the integrands are unbounded on the boundaries of the unit cube. In this thesis we construct function spaces which admit such integrands and present algorithms to construct lattice rules where the worst-case error in this new function space is small.

Lattice rules differ from other quasi-Monte Carlo techniques in that the

points can not be used sequentially. That is, the entire lattice is needed to keep the worst-case error small. It has been shown that there exist generating vectors for lattice rules which are good for many different numbers of points. This is a desirable property for a practitioner, as it allows them to keep increasing the number of points until some error criterion is met. In this thesis, we will develop fast algorithms to construct such generating vectors. Finally, we apply a similar technique to show how a particular type of generating vector known as the *Korobov form* can be made extensible in dimension.

Contents

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Chapter 1

Introduction

This thesis is concerned with the problem of accurately estimating the value of the integral of some function over the d-dimensional unit cube $[0,1]^d$. Such problems are of major interest in areas such as mathematical finance, where the value of the dimension d can be very large. These finance problems typically involve the calculation of some expected value of some payoff function, driven by a random process. The integral is introduced to calculate the expected value of a payoff function where the asset price is assumed to possess some probability distribution. Of course such problems do not arise naturally over the unit cube, as will become apparent later on. However, we will begin by assuming that the integrand is defined over the unit cube.

The Monte Carlo method is a popular approach to estimating the value of the integral. The method involves randomly choosing a number (not necessarily known in advance) of i.i.d. points, say, $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1} \in [0,1]^d$ and evaluating the function at each point. The approximation to the integral is an equal-weight average of the function evaluations. As the value of n increases, the approximation will converge to the true value of the integral.

Quasi-Monte Carlo methods differ from Monte Carlo methods in that rather than being chosen randomly, the points $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}$ are chosen deterministically. While there are many different ways in which this point set may be chosen, we shall be interested in a point sets known as lattice rules. An n-point

point set has points given by $\boldsymbol{t}_k = \{k\boldsymbol{z}/n + \boldsymbol{\Delta}\}$ for $k = 0, 1, \ldots, n-1$, where the integer vector $\boldsymbol{z}$ is known as the generating vector, the vector $\boldsymbol{\Delta}$ is known as the shift, and the braces $\{\cdot\}$ indicate that we are taking only the fractional part. We will always assume that the shift $\boldsymbol{\Delta}$ is randomly chosen from the unit cube $[0,1]^d$. Because of this random shift, we shall refer to our lattice rules as randomly-shifted lattice rules.

We are interested in constructing good randomly-shifted lattice rules. The quality of a randomly-shifted lattice rule for a given value of n is completely determined by the choice of the generating vector $\boldsymbol{z}$. There are many ways to measure the quality of a randomly-shifted point set, or equivalently a generating vector. We will always measure the quality by means of the worst-case error measurement. This quantity for a particular point set $P_{n,d}$ is the greatest difference between the actual value of an integral and its n-point approximation using $P_{n,d}$ taken over all functions in the unit ball of some reproducing kernel Hilbert space. This approach to quality measurement has been extensively studied recently, most commonly with the weighted Korobov and weighted Sobolev spaces being popular choices of reproducing kernel Hilbert spaces. The weights $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ are a set of positive non-increasing weights which correspond to the relative importance of the dimensions.

Analysis of these spaces has proven the existence of lattice rules with small worst-case error and allowed their construction. We will give a more precise definition to the meaning of "small" in due course. It has been shown that if suitable assumptions are made about the weights in the space, then the worst-case error can converge at a rate arbitrarily close to the known optimal rate.

A key weakness with the choice of a weighted Korobov or weighted Sobolev space to measure the worst-case error is that many integrands of interest from the area of mathematical finance do not lie inside the space. This is common because the integrands are typically defined over the whole plane $\mathbb{R}^d$ and then mapped back to the unit cube $[0,1]^d$ via some inverse cumulative density func-

tion. As a result, the integrands are usually unbounded at the boundaries of the unit cube.

The first part of this thesis aims to solve this problem. We introduce reproducing kernel Hilbert spaces which admit integrands unbounded on the boundaries of the unit cube. We show that it is possible to efficiently construct lattice rules, where the number of points is a power of a prime, which have a shift-averaged worst-case error less than the QMC mean. While the rate of convergence is the same as that of the Monte Carlo method and not the optimal rate, numerical results indicate that the lattice rules do in fact achieve close to the optimal rate of convergence. The proof of this remains an open problem.

Most of the material in Chapter 3 is joint work with Ian Sloan and Frances Kuo and appeared in the paper [65]. In that paper, the results were presented for the number of points in the lattice being prime, whereas in the thesis we extend the results to n being a power of a prime. The space introduced in this chapter is a space of analytic functions which possess the boundary behaviour of those unbounded integrands arising from financial applications. We present an algorithm for the construction of lattice rules in this space with small worst-case error. The idea for the inner product of this space came from Ian Sloan. My contribution was the proofs to Lemmas 3.1.1 and 3.2.1, which underpin the proofs of the existence of good lattice rules in the space; I also proved the Theorems 3.2.3 and 3.2.4 which provide a lower and upper bound to the worst case error. I also proved Theorem 3.2.5 which shows that the CBC algorithm does indeed construct a generating vector with worst-case error inside this bound. All of the numerical experiments and programming including the implementation of the fast CBC algorithm were my work as well.

The material in Chapter 4 is joint work with Greg Wasilkowski and Frances Kuo and has appeared in [37]. Again the results in the paper were for n prime, whereas the thesis presents results for n being the power of a prime. Chapter 4 is in many ways an extension of Chapter 3. The space of functions is much

broader, admitting functions whose mixed first derivatives, when multiplied by some weight function ψ_d, are bounded in the L_2-norm. Similar analysis of the space is carried out and a construction algorithm developed for lattice rules with small worst-case error. The idea for the space was due to Greg Wasilkowski. This work was reliant on my proof of Lemma 3.2.1 from the previous chapter, as well as Lemma 4.1.6. I made the suggestion to normalise the worst-case errors by scaling the weights by some constant to allow comparison of worst-case errors with different weights. All of the numerical experiments and programming were my work.

Many of the competing quasi-Monte Carlo alternatives take the form of sequences. That is, the final number of points used in the approximation need not be known in advance. This is an attractive feature because it allows a practitioner to use as many points as required to obtain a given level of accuracy. Since the points in a lattice rule are dependent on the n, the number of points in the lattice must be known in advance. Should the accuracy not be good enough and additional points required, the process must begin again with a different lattice rule and therefore different points. This feature make lattice rules unattractive to a practitioner.

It has been shown that there exist generating vectors $\boldsymbol{z}$ which have small worst-case error for $n = b, b^2, b^3, \ldots$ for any integer $b \geq 2$. Until now, there has been no proven way of constructing such a vector. In Chapter 5 we develop an algorithm to construct generating vectors which achieve the optimal rate of convergence for $n = p^{m_1}, p^{m_1+1}, \ldots, p^{m_2}$ for any prime p and positive integers $m_1 \leq m_2$. This material is joint work with Josef Dick and Friedrich Pillichshammer and will appear in [11]. We will also note how this can be simply extended so that the algorithm works for $n = b^{m_1}, b^{m_1+1}, \ldots, b^{m_2}$ for any integer $b \geq 2$. The initial approach to proving this construction algorithm via a counting argument was developed independently by Friedrich Pillichshammer and myself. Josef Dick made the suggestion of including a probabilistic approach with which we were able to prove that squared worst-case error is

less than some constant times the QMC mean. I also extended the proof to show that the algorithm achieved the optimal rate of convergence. Methods of optimising the performance of the algorithm were my idea. All of the programming and computational results were also my work. The paper [11] also contains an extension of this algorithm for constructing lattice rules with small weighted star-discrepancy which was my work.

Finally, the techniques used in Chapter 5 are also used to construct a Korobov-form generating vector which is extensible in dimension. The existence of such vectors has been known, but these results have until now been non-constructive. This joint work with Josef Dick and Friedrich Pillichshammer forms Chapter 6 and will appear in [12]. My contribution to this work was in the proof that the algorithm described does in fact achieve the optimal rate of convergence. All of the numerical experiments were my work.

Chapter 2

Multivariate integration

This chapter is a summary of the field of multivariate integration. It is intended as a broad introduction to the new material in the following chapters.

We are interested in approximating an integral over the d-dimensional unit cube

$$I_d(f) = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \tag{2.1}$$

with an n-point equal weight quadrature rule of the form

$$Q_{n,d}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f(\boldsymbol{t}_k). \tag{2.2}$$

The point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ consists of points in the d-dimensional unit cube. As will be seen below, we will typically assume that the function f belongs to some reproducing kernel Hilbert space of integrable functions. We are interested primarily in cases where the dimension d is large. Examples of typical problems from mathematical finance (see below in Section 2.7) require d to be in the hundreds, thousands and even larger.

2.1 Monte Carlo and quasi-Monte Carlo

If the points in the point set $P_{n,d}$ are independent and identically distributed random samples from the unit cube, then we shall refer to (2.2) as a *Monte*

Carlo (MC) method. The MC method has the following important classical result.

Theorem 2.1.1 *For all square-integrable functions f*

$$\mathbb{E}[I_d(f) - Q_{n,d}(f)]^2 = \frac{\sigma^2(f)}{n},$$

where the variance of f is given by

$$\sigma^2(f) = I_d(f^2) - [I_d(f)]^2.$$

The MC method has proven very useful for high-dimensional problems because the error bound in Theorem 2.1.1 has convergence of order $\mathcal{O}(n^{-1})$ independent of the dimensional d. Of course the variance $\sigma^2(f)$ may depend on d. However, MC does have three fundamental weaknesses.

The first weakness is the rate of convergence. The error of the MC method converges with order $\mathcal{O}(n^{-1/2})$. We shall see later that it is possible to construct point sets which have a rate of convergence of order $\mathcal{O}(n^{-1})$, or even faster if there is more smoothness present.

The second weakness is the way in which any smoothness in the integrand is ignored. We should exploit the greater levels of smoothness to achieve higher orders of convergence.

Finally, the error bounds achieved by the MC method are probabilistic. It would be preferable to know with certainty that a particular rule has a certain error.

We will attempt to choose point sets $P_{n,d}$ from the unit cube which perform better in the integration problem than MC. Such point sets where the points are chosen in some deterministic manner are known as *quasi-Monte Carlo* (QMC) methods. We shall seek point sets which have a faster rate of convergence than MC, which exploit the smoothness of the integrand and which allow us to determine upper bounds on the error.

2.2 Reproducing kernel Hilbert spaces

We shall see below that it is very often convenient to assume that the function f belongs to a reproducing kernel Hilbert space H_d of integrable functions on $[0,1]^d$. This approach is now widely used in numerical analysis and other areas to define function classes of integrands. The theory of reproducing kernel Hilbert spaces was first developed in [2]. See also [22] where reproducing kernel Hilbert spaces were used to investigate numerical integration.

The reproducing kernel of a reproducing kernel Hilbert space H_d is a function $K_d : [0,1]^d \times [0,1]^d \to \mathbb{R}$ where

$$K_d(\cdot, \boldsymbol{y}) \in H_d \quad \text{for all } \boldsymbol{y} \in [0,1]^d$$

and

$$\langle f, K_d(\cdot, \boldsymbol{y}) \rangle_{H_d} = f(\boldsymbol{y}) \quad \text{for all } \boldsymbol{y} \in [0,1]^d \text{ and } f \in H_d$$

where $\langle \cdot, \cdot \rangle_{H_d}$ denotes the inner product of H_d, and $\|\cdot\|_{H_d} = \langle \cdot, \cdot \rangle_{H_d}^{1/2}$ denotes the corresponding norm.

A reproducing kernel Hilbert space is a Hilbert space were point evaluation is a bounded linear functional on H_d. This is equivalent to assuming that the Hilbert space is equipped with a reproducing kernel. To show this, assume that point evaluation is a bounded linear functional and let

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

For any $\boldsymbol{y} \in [0,1]^d$ by the Riesz representation theorem there exists a unique function $K_d(\cdot, \boldsymbol{y}) \in H_d$, called the *representer* of $T_{\boldsymbol{y}}(f)$, such that for all $\boldsymbol{y} \in [0,1]^d$

$$T_{\boldsymbol{y}}(f) = f(\boldsymbol{y}) = \langle f, K_d(\cdot, \boldsymbol{y}) \rangle_{H_d} \quad \text{for all } f \in H_d. \tag{2.3}$$

Note that any reproducing kernel is symmetric in its arguments, since for all $\boldsymbol{x}, \boldsymbol{y} \in [0,1]^d$

$$K_d(\boldsymbol{x}, \boldsymbol{y}) = \langle K_d(\cdot, \boldsymbol{y}), K_d(\cdot, \boldsymbol{x}) \rangle_{H_d} = \langle K_d(\cdot, \boldsymbol{x}), K_d(\cdot, \boldsymbol{y}) \rangle_{H_d} = K_d(\boldsymbol{y}, \boldsymbol{x}).$$

For any other bounded linear functional T on H_d the representer $\widetilde{T}$ satisfying $T(f) = \left\langle f, \widetilde{T} \right\rangle_{H_d}$ is given by

$$\widetilde{T}(\boldsymbol{y}) = \left\langle \widetilde{T}, K_d(\cdot, \boldsymbol{y}) \right\rangle_{H_d} = \left\langle K_d(\cdot, \boldsymbol{y}), \widetilde{T} \right\rangle_{H_d} = T(K_d(\cdot, \boldsymbol{y})). \tag{2.4}$$

The function spaces we will deal with will always be tensor product spaces. Let $H_1^{(1)}, \ldots, H_1^{(d)}$ be d one-dimensional Hilbert spaces over $[0,1]$, then the tensor product space

$$H_d = H_1^{(1)} \otimes \ldots \otimes H_1^{(d)} \tag{2.5}$$

is the completion of linear combinations of tensor products $f_1 \otimes \cdots \otimes f_d$ where $f_j \in H_1^{(j)}$ for $j = 1, \ldots, d$. The space H_d consists of functions of the form

$$f(\boldsymbol{x}) = \sum_{h_1=1}^{\infty} \cdots \sum_{h_d=1}^{\infty} \left(c_{h_1,\ldots,h_d} \prod_{j=1}^{d} f_{j,h_j}(x_j) \right),$$

where the real coefficients $c_{h_1,\ldots,h_d}$ satisfy

$$\sum_{h_1=1}^{\infty} \cdots \sum_{h_d=1}^{\infty} c_{h_1,\ldots,h_d}^2 < \infty,$$

and for each $j = 1, \ldots, d$, $\{f_{j,h}\}_{h=1}^{\infty}$ forms an orthonormal basis for $H_1^{(j)}$. If each $H_1^{(j)}$ has a reproducing kernel $K_1^{(j)}$, then

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

is the reproducing kernel for H_d.

2.3 Worst-case error analysis

We would like to determine a point set $P_{n,d}$ such that the QMC rule (2.2) is a good approximation to the integral (2.1). We will always perform our analysis in the *worst-case setting*. That is, we will define the *worst-case error* to be

$$e_{n,d}(P_{n,d}; K_d) = \sup_{f \in H_d, \|f\|_{H_d} \le 1} | I_d(f) - Q_{n,d}(f) |,$$

where $P_{n,d}$ is the point set used in (2.2) and K_d is the reproducing kernel of the reproducing kernel Hilbert space H_d. This quantity corresponds to the worst error of the point set over all functions in the unit ball of H_d. We will often compare this to the *initial error* which we define to be

$$e_{0,d}(K_d) = \sup_{f \in H_d, \|f\|_{H_d} \leq 1} |\, I_d(f) \,|\,.$$

2.3.1 Tractability

We will often be interested in reducing the initial error $e_{0,d}$ by some factor. For a reproducing kernel Hilbert space H_d, with reproducing kernel K_d and $\varepsilon \in (0,1)$, we define the minimum number of quadrature points needed to reduce the initial error by a factor of ε^{-1} by

$$n(\varepsilon, d; K_d) = \min\{n : \exists\, P_{n,d} \text{ such that } e_{n,d}(P_{n,d}; K_d) \leq \varepsilon e_{0,d}(K_d)\}.$$

We say that multivariate integration is *QMC tractable* in the space H_d if and only if there exist non-negative constants C, p and q, independent of ε and d such that

$$n(\varepsilon, d; K_d) \leq C\varepsilon^{-p} d^q \quad \text{for all } \varepsilon \in (0,1) \text{ and } d \geq 1.$$

Note that p and q may not be uniquely defined.

We say that multivariate integration is *strongly QMC tractable* in the space H_d if it is QMC tractable with $q = 0$.

In each case, p is known as the ε-exponent of tractability and q is known as the d-exponent of tractability.

2.3.2 Worst-case error formulations

The advantage of considering functions from a reproducing kernel Hilbert space is seen in the following well-known theorem.

Theorem 2.3.1 *The worst-case error for a QMC rule with point set* $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ *in a reproducing kernel Hilbert space* H_d *with reproducing kernel* K_d *where*

$$\int_{[0,1]^{2d}} K_d(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} < \infty \tag{2.6}$$

is given by

$$\begin{aligned} & e^2_{n,d}(P_{n,d}; K_d) \\ &= \int_{[0,1]^{2d}} K_d(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} - \frac{2}{n} \sum_{i=0}^{n-1} \int_{[0,1]^d} K_d(\boldsymbol{t}_i, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{k=0}^{n-1} K_d(\boldsymbol{t}_i, \boldsymbol{t}_k). \end{aligned} \tag{2.7}$$

The initial error satisfies

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

Proof. Due to the assumption (2.6), both I_d and $Q_{n,d}$ are bounded linear functionals on H_d. Using (2.4), we can write

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

where the representer $\xi_{n,d}$ is given by

$$\xi_{n,d} = I_d(K_d(\cdot, \boldsymbol{y})) - Q_{n,d}(K_d(\cdot, \boldsymbol{y})) = \int_{[0,1]^d} K_d(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{n} \sum_{i=0}^{n-1} K_d(\boldsymbol{t}_i, \boldsymbol{y}).$$

The Cauchy-Schwarz inequality gives an error bound of

$$|I_d(f) - Q_{n,d}(f)| = |\langle f, \xi_{n,d} \rangle_{H_d}| \leq \|f\|_{H_d} \|\xi_{n,d}\|_{H_d}.$$

To show that the inequality is sharp, we take f to be $\xi_{n,d}$. In this case, the worst-case error is

$$|I_d(f) - Q_{n,d}(f)| = |\langle \xi_{n,d}, \xi_{n,d} \rangle_{H_d}| = \|\xi_{n,d}\|^2_{H_d}$$

which means that

$$e_{n,d}(P_{n,d}; K_d) = \|\xi_{n,d}\|_{H_d}.$$

We now express the worst-case error in terms of the reproducing kernel K_d for a given point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ by writing

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

The initial error is given by

$$
e^2_{0,d}(K_d) = \left\| \int_{[0,1]^d} K_d(\boldsymbol{x}, \cdot)\, \mathrm{d}\boldsymbol{x} \right\|^2_{H_d} = \int_{[0,1]^{2d}} K_d(\boldsymbol{x}, \boldsymbol{y})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y}.
$$

□

Following [28], we will see that the expression in (2.7) can be simplified if the reproducing kernel is *shift-invariant*. This property means that the reproducing kernel satisfies

$$
K_d(\boldsymbol{x}, \boldsymbol{y}) = K_d(\{\boldsymbol{x} + \boldsymbol{\Delta}\}, \{\boldsymbol{y} + \boldsymbol{\Delta}\}) \text{ for all } \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\Delta} \in [0,1]^d \tag{2.8}
$$

where the braces denote the fractional part of each component of the vector. Taking $\boldsymbol{\Delta} = -\boldsymbol{y}$, we see that for all shift-invariant kernels

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

This allows us to simplify Theorem 2.3.1.

Theorem 2.3.2 *The worst-case error for a QMC rule with point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ in a reproducing kernel Hilbert space H_d with shift-invariant*

reproducing kernel K_d is given by

$$e_{n,d}^2(P_{n,d}; K_d) = -\int_{[0,1]^d} K_d(\boldsymbol{x}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_d(\{\boldsymbol{t}_i - \boldsymbol{t}_k\}, \boldsymbol{0}). \tag{2.9}$$

The initial error satisfies

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

Proof. The proof follows from Theorem 2.3.1 noting that

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

and

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

□

For a point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ and a *shift* $\boldsymbol{\Delta} \in [0,1]^d$, define the *shifted point set* $P_{n,d}(\boldsymbol{\Delta})$ to be the point set with points

$$\{\boldsymbol{t}_0 + \boldsymbol{\Delta}\}, \{\boldsymbol{t}_1 + \boldsymbol{\Delta}\}, \ldots, \{\boldsymbol{t}_{n-1} + \boldsymbol{\Delta}\}.$$

For any reproducing kernel K_d, we define the *associated shift-invariant kernel*, denoted by K_d^{sh}, to be

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

Putting these two concepts together, we obtain the *shift-invariant relationship.*

Theorem 2.3.3 *For any reproducing kernel K_d and associated shift-invariant kernel, and any point set $P_{n,d}$*

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

Proof. We begin by noting that the right-hand side is

$$e^2_{n,d}(P_{n,d};K^{\mathrm{sh}}_d) = -\int_{[0,1]^d} K^{\mathrm{sh}}_d(\boldsymbol{x},\boldsymbol{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K^{\mathrm{sh}}_d(\{\boldsymbol{t}_i-\boldsymbol{t}_k\},\boldsymbol{0})$$

and that

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

Following some manipulations

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

Integration over all possible shifts $\boldsymbol{\Delta}\in[0,1]^d$ gives

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

□

This result will prove to be extremely important. It says that the worst-case error of a shifted point set, averaged over possible shifts, can be explicity written down. This implies that there must exist at least one shift $\boldsymbol{\Delta}$ such that

$$e^2_{n,d}(P_{n,d}(\boldsymbol{\Delta});K_d) \le e^2_{n,d}(P_{n,d};K^{\mathrm{sh}}_d). \tag{2.10}$$

2.3.3 QMC mean

One useful measure of the quality of a point set $P_{n,d}$ is to compare its worst-case error to the *QMC mean*. The QMC mean is defined to be the square root of the average of the squared worst-case error over all possible point sets. Formally, for a reproducing kernel Hilbert space H_d with reproducing kernel K_d we define the QMC mean $M_{n,d}$ by

$$M_{n,d}^2 = \int_{[0,1]^{nd}} e_{n,d}^2(\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}; K_d)\, \mathrm{d}\boldsymbol{t}_0\, \mathrm{d}\boldsymbol{t}_1 \cdots \mathrm{d}\boldsymbol{t}_{n-1}. \tag{2.11}$$

Since $M_{n,d}^2$ represents the average of $e_{n,d}^2(P_{n,d}; K_d)$ over all point sets $P_{n,d}$, we know that there must exist at least one point set $P_{n,d}$ as good as average. That is, at least one point set $P_{n,d}$ where

$$e_{n,d}(P_{n,d}; K_d) \leq M_{n,d}. \tag{2.12}$$

The quantity $M_{n,d}$ can be viewed as an upper bound on the minimal worst-case error.

2.4 Useful spaces

Two of the more commonly examined spaces are the weighted Korobov and weighted Sobolev spaces. In this section we will formally define each space and establish its worst-case error and QMC error. We begin with some brief comments on the weights in these spaces.

2.4.1 Weights

We will see that it is often useful not to assume that each variable is equally important. Sloan and Woźniakowski [56] introduced a non-negative and non-increasing sequence of weights $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ to express the importance of each variable. That is, the weight γ_j symbolises the importance of the j-th variable x_j.

Weights of this type are known as *product weights* and are in fact a subset of the *general weights* $\gamma_{\mathfrak{u}}$ which describes the importance of a set of variables $\boldsymbol{x}_{\mathfrak{u}} = \{x_j : j \in \mathfrak{u}\}$ (see [13, 14, 55]). Other special types of weights include *finite-order weights* and *order-dependent weights*. In this thesis, we will restrict ourselves to the use of product weights.

2.4.2 Weighted Korobov spaces

Here we give an overview of the weighted Korobov space. For a deeper study see [29, 57].

The univariate case

The univariate weighted Korobov space $H_{\mathrm{per},1,\alpha,\gamma}$ is the space of 1-periodic absolutely-integrable functions f on the unit interval with an absolutely convergent Fourier series

$$f(x) = \hat{f}(0) + \sum_{h\in\mathbb{Z}}{}' \hat{f}(h)\mathrm{e}^{2\pi\mathtt{i}hx}$$

and Fourier coefficients

$$\hat{f}(h) = \int_0^1 f(x)\mathrm{e}^{-2\pi\mathtt{i}hx}\,\mathrm{d}x,$$

where $\mathtt{i} = \sqrt{-1}$ and the notation $\sum'$ indicates a summation with the zero term excluded. The inner product of the space $H_{\mathrm{per},1,\alpha,\gamma}$ is given by

$$\begin{aligned}\langle f, g\rangle_{H_{\mathrm{per},1,\alpha,\gamma}} =& \hat{f}(0)\overline{\hat{g}(0)} + \frac{2\pi^2}{\gamma}\sum_{h\in\mathbb{Z}}{}' |h|^\alpha \hat{f}(h)\overline{\hat{g}(h)} \\ =& \sum_{h\in\mathbb{Z}} r_\alpha(h,\gamma)\hat{f}(h)\overline{\hat{g}(h)}\end{aligned}$$

where

$$r_\alpha(h,\gamma) = \begin{cases} 1 & \text{if } h = 0, \\ \frac{2\pi^2|h|^\alpha}{\gamma} & \text{if } h \neq 0. \end{cases}$$

The corresponding norm is given by

$$\|f\|_{H_{\mathrm{per},1,\alpha,\gamma}} = \langle f, f\rangle^{1/2}_{H_{\mathrm{per},1,\alpha,\gamma}} = \left(\sum_{h\in\mathbb{Z}} r_\alpha(h,\gamma)|\hat{f}(h)|^2\right)^{1/2}.$$

The parameter α restricts the convergence of the Fourier coefficients of the functions in the Korobov space. The reproducing kernel of the space $H_{\mathrm{per},1,\alpha,\gamma}$ is given by

$$K_{\mathrm{per},1,\alpha,\gamma}(x,y) = 1 + \frac{\gamma}{2\pi^2} \sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathrm{i} h(x-y)}}{|h|^\alpha} = \sum_{h\in\mathbb{Z}} \frac{\mathrm{e}^{2\pi \mathrm{i} h(x-y)}}{r_\alpha(h,\gamma)}. \tag{2.13}$$

Throughout the thesis we will assume that $\alpha > 1$ so the reproducing kernel is well-defined. The space $H_{\mathrm{per},1,\alpha,\gamma}$ is formally defined to be

$$H_{\mathrm{per},1,\alpha,\gamma} = \{f : \|f\|_{H_{\mathrm{per},1,\alpha,\gamma}} < \infty\}.$$

It is easy to see that $K_{\mathrm{per},1,\alpha,\gamma}$ is a reproducing kernel. We note that for all $y \in [0,1]$ the Fourier coefficients of $K_{\mathrm{per},1,\alpha,\gamma}(\cdot, y)$ are

$$\hat{K}_{\mathrm{per},1,\alpha,\gamma}(h,y) = \frac{\mathrm{e}^{-2\pi \mathrm{i} hy}}{r_\alpha(h,\gamma)}.$$

It follows that for all $f \in H_{\mathrm{per},1,\alpha,\gamma}$

$$\begin{aligned}
\langle f, K_{\mathrm{per},1,\alpha,\gamma}(\cdot,y)\rangle_{H_{\mathrm{per},1,\alpha,\gamma}} &= \sum_{h\in\mathbb{Z}} r_\alpha(h,\gamma)\hat{f}(h)\overline{\hat{K}_{\mathrm{per},1,\alpha,\gamma}(h,y)} \\
&= \sum_{h\in\mathbb{Z}} \hat{f}(h)\mathrm{e}^{2\pi \mathrm{i} hy} \\
&= f(y).
\end{aligned}$$

Remark 2.4.1 The definition given here for the weighted Korobov space differs slightly from the conventional definition in that the weights γ_j are replaced by $\gamma_j/2\pi^2$ for $j = 1, 2, \ldots$. This is done to simplify the relationship between the weighted Korobov space and the weighted Sobolev space as will be seen in Remark 2.4.5.

The multivariate case

As seen in (2.5) of Section 2.2, the d-dimensional weighted Korobov space $H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ is given by

$$H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}} = H_{\mathrm{per},1,\alpha,\gamma_1} \otimes H_{\mathrm{per},1,\alpha,\gamma_2} \otimes \cdots \otimes H_{\mathrm{per},1,\alpha,\gamma_d}.$$

The inner product of the space $H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ is given by

$$\langle f, g\rangle_{H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}} = \sum_{\boldsymbol{h}\in\mathbb{Z}^d} r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})\hat{f}(\boldsymbol{h})\overline{\hat{g}(\boldsymbol{h})},$$

where for $\boldsymbol{h} = (h_1, \ldots, h_d)$,

$$r_\alpha(\boldsymbol{h},\boldsymbol{\gamma}) = \prod_{j=1}^{d} r_\alpha(h_j,\gamma_j).$$

The norm for the d-dimensional case is

$$\|f\|_{H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}} = \langle f, f\rangle^{1/2}_{H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}} = \left(\sum_{\boldsymbol{h}\in\mathbb{Z}^d} r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})|\hat{f}(\boldsymbol{h})|^2\right)^{1/2}.$$

The space $H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ has a reproducing kernel of the form [22]

$$\begin{aligned}
K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) &= \prod_{j=1}^{d} K_{\mathrm{per},1,\alpha,\gamma_j}(x_j, y_j) \\
&= \prod_{j=1}^{d}\left(1 + \frac{\gamma_j}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi\mathrm{i}h(x_j-y_j)}}{|h|^\alpha}\right) \\
&= \prod_{j=1}^{d}\sum_{h\in\mathbb{Z}} \frac{\mathrm{e}^{2\pi\mathrm{i}h(x_j-y_j)}}{r_\alpha(h,\gamma_j)} \\
&= \sum_{\boldsymbol{h}\in\mathbb{Z}^d} \frac{\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}.
\end{aligned} \tag{2.14}$$

The space $H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ is formally defined to be

$$H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}} = \{f : \|f\|_{H_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}} < \infty\}.$$

Worst-case error

Using equations (2.13) and (2.14) we see immediately that the reproducing kernels $K_{\mathrm{per},1,\alpha,\gamma}$ and $K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ are shift-invariant, that is, they satisfy the shift-invariant property given in (2.8). Therefore, using Theorem 2.3.2 and some simple algebraic manipulation we may write the worst-case error for a point

set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ in the d-dimensional Korobov space as

$$\begin{aligned}
&e^2_{n,d}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \\
&= -\int_{[0,1]^d} K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{0})\,\mathrm{d}\boldsymbol{x} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}(\{\boldsymbol{t}_i - \boldsymbol{t}_k\}, \boldsymbol{0}) \\
&= -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1 + \frac{\gamma_j}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi\mathrm{i}h(t_{i,j}-t_{k,j})}}{|h|^\alpha}\right) \qquad (2.15) \\
&= -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}\in\mathbb{Z}^d} \frac{\mathrm{e}^{2\pi\mathrm{i}h\cdot(\boldsymbol{t}_i-\boldsymbol{t}_k)}}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}, \qquad (2.16)
\end{aligned}$$

with the initial error given by $e^2_{0,d}(K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) = 1$.

Upper bounds on the minimal error and the QMC mean

Using (2.11) we see that the QMC mean for the Korobov space is given by

$$\begin{aligned}
M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}} &= \int_{[0,1]^{nd}}\left(-1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}\in\mathbb{Z}^d}\frac{\mathrm{e}^{2\pi\mathrm{i}h\cdot(\boldsymbol{t}_i-\boldsymbol{t}_k)}}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}\right)\mathrm{d}\boldsymbol{t}_0\cdots\mathrm{d}\boldsymbol{t}_{n-1} \\
&= \frac{1}{n}\left(\prod_{j=1}^{d}\left(1 + \frac{\gamma_j\zeta(\alpha)}{\pi^2}\right) - 1\right), \qquad (2.17)
\end{aligned}$$

where $\zeta(\alpha) = \sum_{k=1}^{\infty}\frac{1}{k^\alpha}$ is the Riemann zeta function.

It follows from the averaging argument that there must exist one point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ such that

$$e^2_{n,d}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le \frac{1}{n}\left(\prod_{j=1}^{d}\left(1 + \frac{\gamma_j\zeta(\alpha)}{\pi^2}\right) - 1\right) = M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}. \qquad (2.18)$$

Lower bounds on the minimal error

We have just seen in (2.18) that the upper bound on the minimal error is $M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}$. We will now show that it is possible to get a lower bound on this minimal error.

Theorem 2.4.2 (Sloan and Woźniakowski[57]) *For any point set* $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \ge \frac{1}{n}\prod_{j=1}^{d}\left(1 + \frac{\kappa\gamma_j\zeta(\alpha)}{\pi^2}\right) - 1$$

where

$$\kappa = \min\left(1, \frac{\pi^2}{\gamma_1 |g_{\min}|}\right)$$

and $g_{\min}$ *is the minimum of the function*

$$g(u) = \sum_{h=1}^{\infty} \frac{\cos(2\pi h u)}{|h|^\alpha}, \quad u \in [0,1].$$

Proof. Consider another sequence of non-negative, non-increasing weights $\bar{\boldsymbol{\gamma}} = (\bar{\gamma}_1, \bar{\gamma}_2, \ldots)$ such that $\bar{\gamma}_j \le \gamma_j$ for $j = 1, 2, \ldots$. We see that for all $j = 1, 2, \ldots$ and all $h \in \mathbb{Z}$ that this implies that $r_\alpha(h, \gamma_j) \le r_\alpha(h, \bar{\gamma}_j)$. Using the definition of the norms in the weighted Korobov space, all functions which lie in the unit ball of the space $H_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}$ must also lie in the unit ball of the space $H_{\text{per},d,\alpha,\boldsymbol{\gamma}}$ since

$$\|f\|_{H_{\text{per},d,\alpha,\boldsymbol{\gamma}}} \le \|f\|_{H_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}}, \quad \text{for all } f \in H_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}.$$

By the definition of the worst-case error, we have that

$$e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}) \le e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\boldsymbol{\gamma}}).$$

Also note that

$$g_{\max} = \max_{u \in [0,1]} g(u) = g(0) = \zeta(\alpha).$$

Since there is no value of u such that $\cos(2\pi h u) = -1$ for all $h = 1, 2, \ldots$, it follows that $g_{min} > -g_{\max}$, which implies $|g_{\min}| < g_{\max}$. We see that $K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}(\boldsymbol{x}, \boldsymbol{y})$ can be written as

$$\begin{aligned}
K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}(\boldsymbol{x}, \boldsymbol{y}) &= \prod_{j=1}^{d} \left(1 + \frac{\bar{\gamma}_j}{2\pi^2} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathrm{i} h(x_j - y_j)}}{|h|^\alpha}\right) \\
&= \prod_{j=1}^{d} \left(1 + \frac{\bar{\gamma}_j}{2\pi^2} \sum_{h \in \mathbb{Z}}{}' \frac{\cos(2\pi h(x_j - y_j))}{|h|^\alpha}\right) \\
&= \prod_{j=1}^{d} \left(1 + \frac{\bar{\gamma}_j}{\pi^2} g(x_j - y_j)\right).
\end{aligned}$$

Taking $\bar{\gamma}_j = \kappa \gamma_j$ for all j, we see that each factor $1 + \frac{\bar{\gamma}_j}{\pi^2} g(x_j - y_j)$ is non-negative since,

$$1 + \frac{\bar{\gamma}_j}{\pi^2} g(u) = 1 + \frac{\kappa \gamma_j}{\pi^2} g(u) \ge 1 - \frac{\kappa \gamma_j}{\pi^2} |g_{\min}| \ge 1 - \frac{\kappa \gamma_1}{\pi^2} |g_{\min}| \ge 0$$

and noting that $\cos(x-y) = \cos(|x-y|)$ for all $x, y \in [0,1]$.

Therefore, we can write down the worst-case error of the space $H_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}$ with $\bar{\gamma_j} = \kappa\gamma_j$ to be

$$e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}) = -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}(1 + \frac{\kappa\gamma_j}{\pi^2}g(t_{i,j} - t_{k,j})).$$

Since all the factors in the product are non-negative, we can bound this quantity from below by excluding all the terms where $i \neq k$. This gives us

$$\begin{aligned} e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}) &\geq -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\prod_{j=1}^{d}\left(1 + \frac{\kappa\gamma_j}{\pi^2}g(0)\right) \\ &= \frac{1}{n}\prod_{j=1}^{d}\left(1 + \frac{\kappa\gamma_j\zeta(\alpha)}{\pi^2}\right) - 1. \end{aligned}$$

Since, as shown above, $e_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\bar{\boldsymbol{\gamma}}}) \leq e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\boldsymbol{\gamma}})$, this is also a lower bound to $e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\boldsymbol{\gamma}})$. □

Tractability

In Section 2.3.1 we introduced the concept of tractability. Using the upper and lower bounds on the minimal error found above, we are able to establish sufficient and necessary conditions for tractability and strong tractability in the weighted Korobov space. We defined the quantity

$$n(\varepsilon, d; K_d) = \min\{n : \exists\, P_{n,d} \text{ such that } e_{n,d}(P_{n,d}; K_d) \leq \varepsilon e_{0,d}(K_d)\}$$

which denotes the smallest number of points we require so that there exists a point set where the worst-case error $e_{n,d}(P_{n,d}; K_d)$ is reduced from the initial error $e_{0,d}(K_d)$ by a factor of ε^{-1}, for $\varepsilon \in (0,1)$.

Using the upper bound on $e^2_{n,d}(P_{n,d}; K_{\text{per},d,\alpha,\boldsymbol{\gamma}})$ found in (2.18), and initial error $e_{0,d}(K_{\text{per},d,\alpha,\boldsymbol{\gamma}}) = 1$, we see that

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

implies

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \leq \frac{1}{\varepsilon^2} \prod_{j=1}^{d} \left(1 + \frac{\gamma_j \zeta(\alpha)}{\pi^2}\right).$$

If we use the fact that $\prod_{j=1}^{d} x_j = \exp\left(\sum_{j=1}^{d} \log x_j\right)$, this becomes

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \leq \frac{1}{\varepsilon^2} \exp\left(\sum_{j=1}^{d} \log\left(1 + \frac{\gamma_j \zeta(\alpha)}{\pi^2}\right)\right).$$

Finally, using $\log(1+x) \leq x$ for all $x > -1$ we see that

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \leq \frac{1}{\varepsilon^2} \exp\left(\frac{\zeta(\alpha)}{\pi^2} \sum_{j=1}^{d} \gamma_j\right).$$

Similarly, the lower bound on $e^2_{n,d}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}})$ seen in Theorem 2.4.2 says that

$$e^2_{n,d}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \geq \frac{1}{n} \prod_{j=1}^{d} \left(1 + \frac{\kappa \gamma_j \zeta(\alpha)}{\pi^2}\right) - 1$$

which implies that

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \geq \frac{1}{1+\varepsilon^2} \prod_{j=1}^{d} \left(1 + \frac{\kappa \gamma_j \zeta(\alpha)}{\pi^2}\right),$$

which can be written as

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \geq \frac{1}{1+\varepsilon^2} \exp\left(\sum_{j=1}^{d} \log\left(1 + \frac{\kappa \gamma_j \zeta(\alpha)}{\pi^2}\right)\right).$$

Now, define the function

$$\Psi(x) = \log(1+x) - b_\alpha x, \quad \text{where } b_\alpha = \frac{\log(1 + \kappa\gamma_1\zeta(\alpha)/\pi^2)}{\kappa\gamma_1\zeta(\alpha)/\pi^2}.$$

Clearly

$$\Psi(0) = 0, \quad \Psi(\kappa\gamma_1\zeta(\alpha)/\pi^2) = 0 \quad \text{and } \Psi''(x) = -\frac{1}{(1+x)^2} < 0.$$

Therefore, for all $x \in [0, \kappa\gamma_1\zeta(\alpha)/\pi^2]$, $\log(1+x) \geq b_\alpha x$, which gives

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \geq \frac{1}{1+\varepsilon^2} \exp\left(\frac{b_\alpha \kappa \zeta(\alpha)}{\pi^2} \sum_{j=1}^{d} \gamma_j\right).$$

Putting the upper and lower bounds together, we get

$$\frac{1}{1+\varepsilon^2}\exp\left(\frac{b_\alpha \kappa \zeta(\alpha)}{\pi^2}\sum_{j=1}^{d}\gamma_j\right) \le n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le \frac{1}{\varepsilon^2}\exp\left(\frac{\zeta(\alpha)}{\pi^2}\sum_{j=1}^{d}\gamma_j\right). \tag{2.19}$$

The conditions for tractability and strong tractability can be put in the following theorem.

Theorem 2.4.3 (Sloan and Woźniakowski [57]) *For a sequence of non-increasing, non-negative weights $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$, the integration problem (2.2) in a weighted Korobov space $K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ of functions is*

1. *strongly tractable if and only if*

$$\sum_{j=1}^{\infty}\gamma_j < \infty \tag{2.20}$$

   where the ε-exponent of strong tractability is at most 2,

2. *tractable if and only if*

$$\beta = \limsup_{d\to\infty}\frac{\sum_{j=1}^{d}\gamma_j}{\log(d+1)} < \infty \tag{2.21}$$

   where the ε-exponent of tractability is at most 2 and the d-exponent of tractability can be arbitrarily close to $\zeta(\alpha)\beta/\pi^2$.

Proof. We begin by showing that (2.20) is a sufficient and necessary condition for strong tractability. If $\sum_{j=1}^{\infty}\gamma_j < \infty$, then

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le \frac{1}{\varepsilon^2}\exp\left(\frac{\zeta(\alpha)}{\pi^2}\sum_{j=1}^{\infty}\gamma_j\right) \le C\varepsilon^{-2}$$

for some constant C which is independent of d. This proves the sufficiency of (2.20). If (2.20) does not hold, then the lower bound of (2.19) means that as $d \to \infty$, the quantity $n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \to \infty$, which contradicts strong tractability. Thus (2.20) is a sufficient and necessary condition for strong tractability.

To prove the tractability conditions, we first make use of the observation $\mathrm{e}^x = (d+1)^{x/\log(d+1)}$. This allows us to write (2.19) as

$$\frac{1}{1+\varepsilon^2}(d+1)^{\frac{b_\alpha \kappa \zeta(\alpha)}{\pi^2}\sum_{j=1}^{d}\frac{\gamma_j}{\log(d+1)}} \le n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le \frac{1}{\varepsilon^2}(d+1)^{\frac{\zeta(\alpha)}{\pi^2}\sum_{j=1}^{d}\frac{\gamma_j}{\log(d+1)}}. \tag{2.22}$$

If $\beta = \limsup_{d\to\infty} \frac{\sum_{j=1}^{d}\gamma_j}{\log(d+1)} < \infty$ then for any $\delta > 0$ there exists some d_δ such that

$$\sum_{j=1}^{d}\gamma_j \le (\beta+\delta)\log(d+1), \quad \text{for all } d \ge d_\delta.$$

Therefore, the right-hand inequality of (2.22) implies

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le \varepsilon^{-2}(d+1)^{\frac{\zeta(\alpha)}{\pi^2}(\beta+\delta)}$$

for all $d \ge d_\delta$. So there must exist a constant C_δ such that for all $d \ge 1$,

$$n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \le C_\delta \varepsilon^{-2} d^{\frac{\zeta(\alpha)}{\pi^2}(\beta+\delta)}.$$

Since this holds for any $\delta > 0$, tractability with ε-exponent at most 2 and the d-exponent arbitrarily close to $\zeta(\alpha)\beta/\pi^2$. To prove the necessity, we again observe that if $\beta = \infty$, then by the lower bound of (2.22) with $d \to \infty$, we obtain $n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) \to \infty$ which contradicts tractability. □

2.4.3 Weighted Sobolev spaces

The second space commonly used in the analysis of multivariate integration problems is the weighted Sobolev space. For a deeper look at this space see [53].

The univariate case

The univariate weighted Sobolev space $H_{\mathrm{sob},1,\gamma}$ is the space of absolutely-continuous functions f on the unit interval with square-integrable first derivatives. The inner product of the space $H_{\mathrm{sob},1,\gamma}$ is given by

$$\langle f, g\rangle_{H_{\mathrm{sob},1,\gamma}} = \int_0^1 f(x)\,\mathrm{d}x \int_0^1 g(x) + \frac{1}{\gamma}\int_0^1 f'(x)g'(x)\,\mathrm{d}x.$$

The corresponding norm is given by

$$\|f\|_{H_{\text{sob},1,\gamma}} = \langle f, f\rangle^{1/2}_{H_{\text{sob},1,\gamma}} = \left(\left(\int_0^1 f(x)\,\mathrm{d}x\right)^2 + \frac{1}{\gamma}\int_0^1 f'(x)^2\,\mathrm{d}x\right)^{1/2}$$

and the reproducing kernel of the space $H_{\text{sob},1,\gamma}$ is

$$K_{\text{sob},1,\gamma}(x,y) = 1 + \gamma\left(\tfrac{1}{2}B_2\left(|x-y|\right) + (x-\tfrac{1}{2})(y-\tfrac{1}{2})\right) \tag{2.23}$$

The function $B_2(x) = x^2 - x + \frac{1}{6}, x \in [0,1]$ is the Bernoulli polynomial of degree 2. It is sometimes convenient to use the form

$$B_2(x) = \frac{1}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} h x}}{h^2}, \quad x \in [0,1]. \tag{2.24}$$

The space $H_{\text{sob},1,\gamma}$ is formally defined to be

$$H_{\text{sob},1,\gamma} = \{f : \|f\|_{H_{\text{sob},1,\gamma}} < \infty\}.$$

Remark 2.4.4 This particular Sobolev space is known as the *unanchored* Sobolev space. Similar *anchored* Sobolev spaces can be constructed with the inner product of the form

$$\langle f, g\rangle_{H_{\text{sob},1,\gamma}} = f(a)g(a) + \frac{1}{\gamma}\int_0^1 f'(x)g'(x)\,\mathrm{d}x \tag{2.25}$$

for some $a \in [0,1]$ (see [53]). The reproducing kernel for the space $H_{\text{sob},1,\gamma}$ in this case is

$$K_{\text{sob},1,\gamma}(x,y) = 1 + \gamma\omega_a(x,y)$$

where

$$\omega_a(x,y) = \begin{cases} \min(|x-a|, |y-a|), & \text{if } (x-a)(y-a) > 0, \\ 0, & \text{if } (x-a)(y-a) \le 0. \end{cases}$$

Throughout this thesis, we will adopt the unanchored version, in order to simplify the algebra.

It is easy to see that $K_{\text{sob},1,\gamma}$ is a reproducing kernel. Note that

$$\tfrac{1}{2}B_2\left(|x-y|\right) + (x-\tfrac{1}{2})(y-\tfrac{1}{2}) = \begin{cases} \frac{1}{2}x^2 + \frac{1}{2}y^2 - y + \frac{1}{3}, & \text{if } 0 \le x \le y, \\ \frac{1}{2}x^2 + \frac{1}{2}y^2 - x + \frac{1}{3}, & \text{if } y < x \le 1, \end{cases}$$

so that $\int_0^1 \frac{1}{2}B_2\left(|x-y|\right) + (x-\frac{1}{2})(y-\frac{1}{2})\,\mathrm{d}x = 0$. Also note that

$$\frac{\partial}{\partial x}\left(\tfrac{1}{2}B_2\left(|x-y|\right) + (x-\tfrac{1}{2})(y-\tfrac{1}{2})\right) = \begin{cases} x, & \text{if } 0 \le x < y, \\ -1+x, & \text{if } y < x \le 1, \end{cases}$$

It follows with some simple manipulation that for all $f \in H_{\mathrm{sob},1,\gamma}$

$$\langle f, K_{\mathrm{sob},1,\gamma}(\cdot, y)\rangle_{H_{\mathrm{sob},1,\gamma}} = f(y)$$

thus proving the reproducing property.

Unlike the kernel of the Korobov space $H_{\mathrm{per},1,\alpha,\gamma}$, the kernel of the space $H_{\mathrm{sob},1,\gamma}$ is not shift-invariant. With some manipulation, we see that the associated shift-invariant kernel $K^{\mathrm{sh}}_{\mathrm{sob},1,\gamma}$ is given by

$$K^{\mathrm{sh}}_{\mathrm{sob},1,\gamma}(x,y) = \int_0^1 K_{\mathrm{sob},1,\gamma}(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta = 1 + \gamma B_2\left(|x-y|\right).$$

Remark 2.4.5 Since $B_2\left(|x-y|\right) = B_2\left(\{x-y\}\right)$ for all $x, y \in [0,1]$, we can use (2.24) to see that the associated shift-invariant kernel of the weighted Sobolev space $K^{\mathrm{sh}}_{\mathrm{sob},1,\gamma}$ is identical to the reproducing kernel of the weighted Korobov space $K_{\mathrm{per},1,\alpha,\gamma}$ given in (2.13) with $\alpha = 2$. Note also that the representer of integration is the function $K_{\mathrm{sob},1,\gamma}(\cdot, y) = 1$.

The multivariate case

The multivariate weighted Sobolev space $H_{\mathrm{sob},d,\boldsymbol{\gamma}}$ is given by

$$H_{\mathrm{sob},d,\boldsymbol{\gamma}} = H_{\mathrm{sob},1,\gamma_1} \otimes H_{\mathrm{sob},1,\gamma_2} \otimes \cdots \otimes H_{\mathrm{sob},1,\gamma_d}.$$

The inner product of the space $H_{\mathrm{sob},d,\boldsymbol{\gamma}}$ is given by

$$\langle f, g\rangle_{H_{\mathrm{sob},d,\gamma}} = \sum_{\mathfrak{u}\subseteq\mathcal{D}} \left(\prod_{j\in\mathfrak{u}} \frac{1}{\gamma_j} \int_{[0,1]^{\mathfrak{u}}} \left(\int_{[0,1]^{d-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} f}{\partial \boldsymbol{x}_{\mathfrak{u}}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}_{\mathcal{D}\setminus\mathfrak{u}} \right) \times \left(\int_{[0,1]^{d-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} g}{\partial \boldsymbol{x}_{\mathfrak{u}}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}_{\mathcal{D}\setminus\mathfrak{u}} \right) \mathrm{d}\boldsymbol{x}_{\mathfrak{u}} \right) \quad (2.26)$$

where we define $\mathcal{D} = \{1, 2, \ldots, d\}$, $|\mathfrak{u}|$ denotes the cardinality of $\mathfrak{u}$, $\boldsymbol{x}_{\mathfrak{u}}$ is the $|\mathfrak{u}|$-dimensional vector with components of $\boldsymbol{x}$ whose indices belong to $\mathfrak{u}$ and

$\boldsymbol{x}_{\mathcal{D}\setminus\mathfrak{u}}$ denotes the $(d-|\mathfrak{u}|)$-dimensional vector with components of $\boldsymbol{x}$ whose indices do not belong to $\mathfrak{u}$. The norm for the d-dimensional case is

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

The space $H_{\mathrm{sob},d,\boldsymbol{\gamma}}$ has a reproducing kernel of the form

$$K_{\mathrm{sob},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d} \left(1+\gamma_j \left(\tfrac{1}{2}B_2\left(|x_j-y_j|\right) + (x_j-\tfrac{1}{2})(y_j-\tfrac{1}{2})\right)\right). \qquad (2.27)$$

The space $H_{\mathrm{sob},d,\boldsymbol{\gamma}}$ is formally defined to be

$$H_{\mathrm{sob},d,\boldsymbol{\gamma}} = \{f : \|f\|_{H_{\mathrm{sob},d,\boldsymbol{\gamma}}} < \infty\}.$$

The associated shift-invariant kernel $K^{\mathrm{sh}}_{\mathrm{sob},d,\boldsymbol{\gamma}}$ is

$$K^{\mathrm{sh}}_{\mathrm{sob},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d} \left(1+\gamma_j B_2\left(|x_j-y_j|\right)\right)$$

and is again identical to the kernel $K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}$ with $\alpha = 2$. Note that the representer of multivariate integration is the function $K_{\mathrm{sob},1,\gamma}(\cdot,\boldsymbol{y}) = 1$.

Worst-case error and QMC mean

Since the kernel $K_{\mathrm{sob},d,\boldsymbol{\gamma}}$ is not shift-invariant, we need to use Theorem 2.3.1 to evaluate the worst-case error of a given point set $P_{n,d} = \{\boldsymbol{t}_0,\boldsymbol{t}_1,\ldots,\boldsymbol{t}_{n-1}\}$. Following some manipulation we get

$$\begin{aligned} &e^2_{n,d}(P_{n,d};K_{\mathrm{sob},d,\boldsymbol{\gamma}}) \\ &= -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1+\gamma_j\left(\tfrac{1}{2}B_2\left(|t_{i,j}-t_{k,j}|\right)+(t_{i,j}-\tfrac{1}{2})(t_{k,j}-\tfrac{1}{2})\right)\right) \end{aligned}$$

and the initial error is given by $e^2_{0,d}(K_{\mathrm{sob},d,\boldsymbol{\gamma}}) = 1$. Using Theorem 2.3.3 we see that error of a shifted point set $P_{n,d}(\boldsymbol{\Delta}) = \{\{\boldsymbol{t}_0+\boldsymbol{\Delta}\},\{\boldsymbol{t}_1+\boldsymbol{\Delta}\},\ldots,\{\boldsymbol{t}_{n-1}+\boldsymbol{\Delta}\}\}$, averaged over all possible shifts $\boldsymbol{\Delta}\in[0,1]^d$ is given by

$$\begin{aligned} \int_{[0,1]^d} e^2_{n,d}(P_{n,d}(\boldsymbol{\Delta});K_{\mathrm{sob},d,\boldsymbol{\gamma}})\,\mathrm{d}\boldsymbol{\Delta} &= e^2_{n,d}(P_{n,d};K^{\mathrm{sh}}_{\mathrm{sob},d,\boldsymbol{\gamma}}) \\ &= 1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1+\gamma_j B_2\left(|t_{i,j}-t_{k,j}|\right)\right). \end{aligned}$$

Using (2.11) we see that the QMC mean for the Sobolev space is given by

$$M^2_{\mathrm{sob},n,d,\boldsymbol{\gamma}} = \frac{1}{n}\left(\prod_{j=1}^{d}\left(1+\frac{\gamma_j}{6}\right)-1\right),$$

which, as expected, is exactly the same as the QMC mean for the weighted Korobov space in 2.17 with $\alpha = 2$. Note that $\zeta(2) = \frac{\pi^2}{6}$. Further, it is clear that the analogue of Theorem 2.4.3 for the Sobolev space is identical with $\alpha = 2$.

2.4.4 Randomly shifted point sets

We will see below that point sets $P_{n,d}(\boldsymbol{\Delta})$, where the shift $\boldsymbol{\Delta}$ is taken to be randomly from a uniform distribution over the unit cube $[0,1]^d$, are particularly interesting. Theorem 2.3.3 says that the average worst case error of a shifted point set in a weighted Sobolev space, averaged over all possible shifts, is equal to the worst-case error of the unshifted point set in the weighted Korobov space with $\alpha = 2$.

This means we can say that the *expected* worst-case error in a weighted Sobolev space for a randomly shifted point set is identical to the error of the unshifted point set in the weighted Korobov space with $\alpha = 2$. That is

$$\mathbb{E}\left[e_{n,d}(P_{n,d}(\boldsymbol{\Delta}); K_{\mathrm{sob},d,\boldsymbol{\gamma}})\right] = e_{n,d}(P_{n,d}; K^{\mathrm{sh}}_{\mathrm{sob},d,\boldsymbol{\gamma}}) = e_{n,d}(P_{n,d}; K_{\mathrm{per},d,2,\boldsymbol{\gamma}}). \quad (2.28)$$

Therefore, while we will from now on mainly refer to point sets in the weighted Korobov space, all the results carry over in a probabilistic sense for randomly-shifted point sets in the weighted Sobolev space when we take $\alpha = 2$.

It is of course possible to check the quality of a particular shift by computing the worst-case error. Therefore, we have can create a "semi-constructive" approach to finding shifts $\boldsymbol{\Delta}$ which such that

$$e_{n,d}(P_{n,d}(\boldsymbol{\Delta}); K_{\mathrm{sob},d,\boldsymbol{\gamma}}) \leq c e_{n,d}(P_{n,d}; K^{\mathrm{sh}}_{\mathrm{sob},d,\boldsymbol{\gamma}})$$

for some $c > 1$. By Chebyshev's inequality, taking s random shifts will generate at least one such shift with probability $1 - c^{-s}$.

2.4.5 Unbiased error estimation

We would like to be able to measure the performance of a particular point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ on a particular problem. We will do this by calculating an unbiased estimate of the standard error of an average of several evaluations using different random shifts.

For a particular problem $I_d(f)$ of the form (2.1), and an unshifted point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$, we generate s random shifts $\boldsymbol{\Delta}_1, \ldots, \boldsymbol{\Delta}_s$ each i.i.d. from $[0,1]^d$ to construct the shifted point sets $P_{n,d}(\boldsymbol{\Delta}_1), \ldots, P_{n,d}(\boldsymbol{\Delta}_s)$. We then evaluate for $\ell = 1, \ldots, s$

$$Q_{\ell,n,d} = \frac{1}{n}\sum_{k=0}^{n-1} f(\boldsymbol{t}_{\ell,k}), \quad \text{where } \boldsymbol{t}_{\ell,k} = \{\boldsymbol{t}_k + \boldsymbol{\Delta}_\ell\}.$$

We then approximate $I_d(f)$ by

$$\overline{Q}_{n,d} = \frac{1}{s}\sum_{\ell=1}^{s} Q_{\ell,n,d}.$$

An unbiased estimate of the standard error of $\overline{Q}_{n,d}$ is

$$\sqrt{\frac{1}{s(s-1)}\sum_{\ell=1}^{s}(Q_{\ell,n,d} - \overline{Q}_{n,d})^2}.$$

2.5 Lattice rules

We aim to find a good point set $P_{n,d} = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$, or shifted point set $P_{n,d}(\boldsymbol{\Delta}) = \{\{\boldsymbol{t}_0 + \boldsymbol{\Delta}\}, \{\boldsymbol{t}_1 + \boldsymbol{\Delta}\}, \ldots, \{\boldsymbol{t}_{n-1} + \boldsymbol{\Delta}\}\}$, which will accurately approximate the integration problem (2.1) when used as quadrature points in the QMC method (2.2). The results so far in this chapter have provided us with tools to examine the worst-case error for a given (possibly randomly-shifted) point set in a reproducing kernel Hilbert space. The problem remains to choose the set of points $P_{n,d}$.

There are many possible choices of $P_{n,d}$. It is beyond the scope of this thesis to give a summary of all of them. Some of the more popular choices of

quadrature points are Halton sequences [18], Hammersley point sets [19], Sobol' points [58], Niederreiter-Xing sequences [66], (t, d)-sequences and (t, m, d)-nets [41, 42, 44]. The remainder of the thesis will concentrate on a particular choice of point sets known as *lattice rules*.

Definition 2.5.1 *A rank-1 lattice rule is an equal-weight quadrature rule of the form*

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

where $\boldsymbol{z} \in \{1, 2, \ldots, n-1\}^d$ *is called the generating vector with* $\gcd(z_j, n) = 1$ *for all* $j = 1, \ldots, d$. *The points*

$$\boldsymbol{t}_k = \left\{ \frac{k\boldsymbol{z}}{n} \right\}, \quad k = 1, \ldots n$$

are known as (unshifted) lattice points. The set $P_{n,d}(\boldsymbol{z}) = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ *defines the (unshifted) point set which is wholly determined by the generating vector* $\boldsymbol{z}$.

Lattice rules in their early form were first analysed by Korobov [33] and Hlawka [30]. A textbook have been written by Sloan and Joe in 1994 [51]. Lattice rules were also mentioned in the book by Niederreiter in 1992 [42].

One of the key advantages of lattice rules lies in the one-dimensional projections. It is well-known that for one-dimensional integration on the unit interval with equal-weight quadrature points, the optimal choice for points is equally-spaced points. In this sense, all lattice rules have optimal one-dimensional projections.

We will see that the family of *shifted rank-1 lattice rules* is also particularly interesting.

Definition 2.5.2 *A shifted rank-1 lattice rule is an equal-weight quadrature rule of the form*

$$Q_{n,d}(f) = \frac{1}{n} \sum_{k=0}^{n-1} f\left(\left\{ \frac{k\boldsymbol{z}}{n} + \boldsymbol{\Delta} \right\} \right). \tag{2.29}$$

The set $P_{n,d}(\boldsymbol{z}, \boldsymbol{\Delta}) = \{\{\boldsymbol{t}_0 + \boldsymbol{\Delta}\}, \{\boldsymbol{t}_1 + \boldsymbol{\Delta}\}, \ldots, \{\boldsymbol{t}_{n-1} + \boldsymbol{\Delta}\}\}$*, where* $\boldsymbol{t}_k = \left\{\frac{k\boldsymbol{z}}{n}\right\}$ *for* $k = 1, \ldots n$*, defines the point set of shifted lattice points and is determined by the generating vector* $\boldsymbol{z}$ *and the shift* $\boldsymbol{\Delta} \in [0,1]^d$*.*

2.5.1 Worst-case error formulation

In this thesis, we will concern ourselves with point sets consisting of randomly shifted lattice rules. We will therefore now drop the $P_{n,d}$ notation, expressing the worst-case error for a lattice rule in a Korobov space as $e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$. The worst-case error for a lattice rule with a given shift $\boldsymbol{\Delta}$ in the Sobolev space is denoted by $e_{\mathrm{sob},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}, \boldsymbol{\Delta})$ and the expected error for a randomly-shifted lattice is given by $e_{\mathrm{sob},n,d,\boldsymbol{\gamma}}(\boldsymbol{z})$. Under this notation, taking $\alpha = 2$, (2.28) becomes

$$\mathbb{E}\left[e_{\mathrm{sob},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}, \boldsymbol{\Delta})\right] = e_{\mathrm{sob},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}) = e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}).$$

We have seen above in (2.15) and (2.16) that the worst case error of a point set in a Korobov space can be written as

$$\begin{aligned} e^2_{n,d}(P_{n,d}; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}}) &= -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1 + \frac{\gamma_j}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathrm{i} h(t_{i,j}-t_{k,j})}}{|h|^\alpha}\right) \\ &= -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}\in\mathbb{Z}^d} \frac{\mathrm{e}^{2\pi \mathrm{i}\boldsymbol{h}\cdot(\boldsymbol{t}_i-\boldsymbol{t}_k)}}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})} \end{aligned}$$

This formulation requires a double sum each over n terms. This is unattractive from a computational perspective as the number of points n can become very large. However, if we exploit the structure in the rank-1 lattice rule with points

$$\boldsymbol{t}_k = \left\{\frac{k\boldsymbol{z}}{n}\right\}, \quad \text{for } k = 0, \ldots n-1$$

we see that the expressions in (2.15) and (2.16) simplify to

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) = -1 + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1 + \frac{\gamma_j}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathrm{i} k h z_j/n}}{|h|^\alpha}\right) \tag{2.30}$$

$$= -1 + \frac{1}{n}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}\in\mathbb{Z}^d} \frac{\mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n}}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}$$

$$= \sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^d\setminus\{\boldsymbol{0}\} \\ \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n}} \frac{1}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}. \tag{2.31}$$

The final line (2.31) follows from the result

$$\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n} = \begin{cases} 1 & \text{if } \boldsymbol{h}\cdot\boldsymbol{z} \equiv 0 \pmod{n}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.32}$$

From a computational perspective if $\alpha = 2$, then using the Bernoulli polynomial from (2.24), the formulation in (2.30) is the most useful, as it requires just a single sum over n terms. The form in (2.31) will prove useful later on.

2.5.2 Existence of good lattice rules

Recall that the components of the vector $\boldsymbol{z} \in \{1, \ldots, n-1\}^d$ must be co-prime with n. For simplicity, it is often assumed that n is prime. It turns out that the formulations are also relatively simple if n is taken to be the power of a prime. In this thesis, we will usually assume that n is indeed the power of a prime, although we see that the results in Chapter 5 can be extended to n being the power of an arbitrary positive integer. For results concerning lattice rules for more general composite numbers n, the reader is directed to [36]. We now define formally the sets of vectors which may be considered as admissible generating vectors for n being prime or, more generally, a power of a prime of the form $n = p^m$, where p is prime and m some non-negative integer. We first define the set of d-dimensional integer vectors with components co-prime to $n = p^m$

$$\mathcal{Z}_p^d = \{\boldsymbol{z} = (z_1, \ldots, z_d) \in \mathbb{N}^d : \gcd(z_j, p^m) = 1, j = 1, \ldots, d\}, \tag{2.33}$$

where $\mathbb{N} = \{1, 2, \ldots\}$. The set of admissible generating vectors is then given by

$$\mathcal{Z}_{p,m}^d = \{\boldsymbol{z} \in \mathcal{Z}_p^d : z_j < p^m, j = 1, \ldots, d\}. \tag{2.34}$$

For analysis of convergence, it is often easier to think in terms of n, rather than p^m. Therefore, we will take the set $\mathcal{Z}_{n,1}^d$ to mean the same as $\mathcal{Z}_{p,m}^d$ where $n = p^m$. In cases where $d = 1$, we may drop the superscript. Note that the cardinality of the set $\mathcal{Z}_{p,m}^d = \phi(p^m)^d$, where ϕ is Euler's totient function; and

$\phi(p^m) = p^{m-1}(p-1)$ is p is prime. For the remainder of the thesis, unless otherwise stated, we will always assume that p prime.

We now show that there exist *good* generating vectors $\boldsymbol{z}$. At this stage, we will say a generating vector is "good" (or equivalently that the worst-case error is "small") if the worst-case error of the lattice rule it generates is less than the QMC mean as defined in (2.11).

Theorem 2.5.3 *Let m and d be positive integers and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ a positive non-increasing sequence. If $p \geq \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ then we have*

$$\frac{1}{\phi(p^m)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_{p,m}^d} e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}$$

where $M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}$ is the QMC mean of the weighted Korobov space as given in (2.17).

Proof. The proof of the first part is similar to the proof of [36, Theorem 2.2]. We see that

$$\begin{aligned}
&\frac{1}{\phi(p^m)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_{p,m}^d} e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \\
&= -1 + \frac{1}{p^m} \prod_{j=1}^{d} \left(1 + \frac{\gamma_j \zeta(\alpha)}{\pi^2}\right) \\
&\quad + \frac{1}{p^m} \sum_{k=1}^{p^m} \prod_{j=1}^{d} \left(1 + \frac{1}{\phi(p^m)} \frac{\gamma_j}{2\pi^2} \sum_{z_j \in \mathcal{Z}_{p,m}} {\sum_{h \in \mathbb{Z}}}' \frac{\mathrm{e}^{2\pi \mathrm{i} k h z_j / p^m}}{|h|^\alpha}\right) \\
&\leq M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}},
\end{aligned}$$

where the final inequality holds if

$$\prod_{j=1}^{d} \left(1 + \frac{1}{\phi(p^m)} \frac{\gamma_j}{2\pi^2} \sum_{z_j \in \mathcal{Z}_{p,m}} {\sum_{h \in \mathbb{Z}}}' \frac{\mathrm{e}^{2\pi \mathrm{i} k h z_j / p^m}}{|h|^\alpha}\right) \leq 1.$$

We will show that this does indeed hold if $p \geq \frac{1}{\alpha} \log\left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)$ by showing that for all $j = 1, \ldots, d$ and $k = 1, \ldots, p^m - 1$

$$-1 \leq 1 + \frac{1}{\phi(p^m)} \frac{\gamma_j}{2\pi^2} \sum_{z_j \in \mathcal{Z}_{p,m}} {\sum_{h \in \mathbb{Z}}}' \frac{\mathrm{e}^{2\pi \mathrm{i} k h z_j / p^m}}{|h|^\alpha} \leq 1.$$

By [36, Lemma 2.1] we see that

$$\frac{1}{\phi(p^m)} \sum_{z_j \in \mathcal{Z}_{p,m}} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z_j / p^m}}{|h|^\alpha} = \frac{2\zeta(\alpha)}{\phi(p^m)} \frac{\gcd(p^{m-1}, k)^\alpha}{(p^m)^{\alpha-1}} \left(1 - p^{\alpha-1}\right) < 0$$

which takes care of the second inequality. Using [36, Lemma 2.1] again we see that the first inequality will hold if

$$\frac{1}{\phi(p^m)} \frac{\gcd(p^{m-1}, k)^\alpha}{(p^m)^{\alpha-1}} \left(p^{\alpha-1} - 1\right) \le \frac{2\pi^2}{\gamma_j \zeta(\alpha)} \tag{2.35}$$

for each $k = 1, \ldots, p^m - 1$. For a given k, take $\gcd(p^{m-1}, k) = p^\ell$. Now, using $\phi(p^m) = p^{m-1}(p-1)$ for p prime, we see that (2.35) will hold if for all $\ell = 0, 1, \ldots, m-1$

$$\left(p^{m-\ell}\right)^\alpha \ge \frac{\gamma_j \zeta(\alpha)}{2\pi^2}.$$

This holds for all the required values of ℓ if $p \ge \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$, since $\gamma_1 \ge \gamma_2 \ge \cdots$. □

Remark 2.5.4 The constraint on the choice of p is not great since it will always be satisfied if $\alpha = 2$ and $\gamma_1 \le 12$.

Theorem 2.5.3 says that the average squared worst-case error taken over *all* choices of admissible generating vectors is less than the square of the QMC mean. Using an averaging argument, this theorem admits a simple corollary.

Corollary 2.5.5 *Let $n = p^m$ be a power of a prime p such that $p \ge \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ and d be a positive integer. There exists at least one $\boldsymbol{z} \in \mathcal{Z}_{n,1}^d$ such that*

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}} = \frac{1}{n} \left(\prod_{j=1}^{d} \left(1 + \frac{\gamma_j \zeta(\alpha)}{\pi^2}\right) - 1 \right).$$

Corollary 2.5.6 *For $n = p^m$ with $p \ge \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$, if $\sum_{j=1}^{\infty} \gamma_j < \infty$ then there exists a generating vector $\boldsymbol{z}$ and a constant C_∞ independent of d such that*

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le C_\infty n^{-1/2}.$$

Proof. We have seen from Corollary 2.5.5 that there exists

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le C_d n^{-1/2}. \tag{2.36}$$

Once again using $\log(1+x) \le x$ for $x > -1$ we get

$$\begin{aligned} C_d^2 = \left(\prod_{j=1}^{d}\left(1+\frac{\gamma_j\zeta(\alpha)}{\pi^2}\right)-1\right) &\le \exp\left(\sum_{j=1}^{d}\log\left(1+\frac{\gamma_j\zeta(\alpha)}{\pi^2}\right)\right) \\ &\le \exp\left(\frac{\zeta(\alpha)}{\pi^2}\sum_{j=1}^{d}\gamma_j\right) \\ &\le \exp\left(\frac{\zeta(\alpha)}{\pi^2}\sum_{j=1}^{\infty}\gamma_j\right) = C_\infty^2, \end{aligned}$$

where C_∞ is independent of d if $\sum_{j=1}^{\infty}\gamma_j < \infty$. □

Note that the condition $\sum_{j=1}^{\infty}\gamma_j < \infty$ is exactly the sufficient and necessary condition for strong tractability in Section 2.4.2.

To achieve a similar result to Theorem 2.5.3 without the constraint on the prime p, we note the following theorem from Kuo and Joe [36, Theorem 2.2].

Theorem 2.5.7 *Let m and d be positive integers, p prime and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ a positive non-increasing sequence. Then we have*

$$\frac{1}{\phi(p^m)^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_{p,m}^d} e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}} \tag{2.37}$$

where

$$\overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}} = \frac{1}{p^m}\left(\prod_{j=1}^{d}\left(1+4\frac{\gamma_j}{2\pi^2}\zeta(\alpha)\right)-1\right) \tag{2.38}$$

Remark 2.5.8 Note that the proof of Theorem 2.5.7 as given in [36] unnecessarily omits the final -1 term in (2.38).

Remark 2.5.9 The result in [36] in fact gives a more general result for n being an arbitrary positive integer. In this case we can generalise (2.38) by replacing $\overline{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}$ with $\widetilde{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}$ where

$$\widetilde{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}} = \frac{1}{n}\left(\prod_{j=1}^{d}\left(1+2^{\kappa+1}\frac{\gamma_j}{2\pi^2}\zeta(\alpha)\right)-1\right) \tag{2.39}$$

and κ is the number of distinct prime factors of n. We will continue to assume that $n = p^m$ is the power of a prime p, but will point out in Chapter 5 where this can be easily generalised.

2.5.3 Optimal rate of convergence

Recall earlier from Theorem 2.1.1 that the expected error of MC integration is $\mathcal{O}(n^{-1/2})$. From Corollary 2.5.6 we see that if

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

then the worst-case error, where n is the power of a prime, is also $\mathcal{O}(n^{-1/2})$. It is also known classically that the best rate of convergence possible for a one-dimensional problem is $\mathcal{O}(n^{-\alpha/2})$, known as the *optimal rate of convergence*. Clearly, if this is the best possible for a one-dimensional problem, then it must also give an upper bound for problems of higher dimension. We will now see that if we impose stronger conditions on the weights, it is possible to achieve this rate of convergence using lattice rules for problems of arbitrary dimension.

Theorem 2.5.10 *Let $n = p^m$ be the power of a prime p with $p \geq \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ a positive non-increasing sequence where (2.20) holds, then there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_{n,1}^d$ such that for all $\lambda \in (1/\alpha, 1]$*

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda),$$

where

$$M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) = n^{-1/\lambda} \left(\prod_{j=1}^{d} \left(1 + 2 \left(\frac{\gamma_j}{2\pi^2} \right)^{\lambda} \zeta(\alpha\lambda) \right) - 1 \right)^{1/\lambda}.$$

Further, if

$$s^* = \sup \left\{ s : \sum_{j=1}^{\infty} \gamma_j^{1/s} < \infty \right\}, \tag{2.40}$$

then the integration problem is strongly tractable with the ε-exponent of strong tractability lying in the range $(\frac{2}{\alpha}, \max(\frac{2}{s^*}, \frac{2}{\alpha})]$.

Proof. The result is roved by making use of Jensen's inequality, which states for a sequence $\{a_k\}$ of positive numbers

$$\sum_k a_k \le \left(\sum_k a_k^\lambda\right)^{1/\lambda} \quad \text{for all } 0 < \lambda \le 1. \tag{2.41}$$

Applying Jensen's inequality to $e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$, using the formulation in (2.31), note that $[r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})]^\lambda = r_{\alpha\lambda}(\boldsymbol{h}, 2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda)$, where $(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda = ((\frac{\gamma_1}{2\pi^2})^\lambda, (\frac{\gamma_2}{2\pi^2})^\lambda, \ldots)$. This implies that for any $\boldsymbol{z} \in \mathcal{Z}^d_{n,1}$ and for all $0 < \lambda \le 1$ we obtain

$$\begin{aligned} e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) &\le \left(\sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^d\setminus\{\boldsymbol{0}\}\\ \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n}} \frac{1}{[r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})]^\lambda}\right)^{1/\lambda} \\ &= \left(\sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^d\setminus\{\boldsymbol{0}\}\\ \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n}} \frac{1}{r_{\alpha\lambda}(\boldsymbol{h}, 2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda)}\right)^{1/\lambda} \\ &= [e^2_{\text{per},n,d,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}(\boldsymbol{z})]^{1/\lambda}. \end{aligned} \tag{2.42}$$

Now from Corollary 2.5.5 we see that for $n = p^m$, the power of a prime p where $p \ge \left(\frac{\gamma_1\zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$, there exists a $\boldsymbol{z} \in \mathcal{Z}^d_{n,1}$ such that

$$e^2_{\text{per},n,d,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}(\boldsymbol{z}) \le \frac{1}{n}\left(\prod_{j=1}^d \left(1 + 2\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda \zeta(\alpha\lambda)\right) - 1\right).$$

We see from (2.42) that this implies that there exists a $\boldsymbol{z} \in \mathcal{Z}^d_{n,1}$ such that for all $\lambda \in (1/\alpha, 1]$

$$e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le n^{-1/\lambda}\left(\prod_{j=1}^d \left(1 + 2\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda \zeta(\alpha\lambda)\right) - 1\right)^{1/\lambda}.$$

Note that we must restrict the range of values λ so that $\zeta(\alpha\lambda)$ is well defined, i.e. $\lambda\alpha > 1$. To see that the integration problem is strongly tractable, we recall (2.36) and write

$$e_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le C_{d,\lambda} n^{-1/2\lambda},$$

where

$$C_{d,\lambda} = \left(\prod_{j=1}^{d} \left(1 + 2 \left(\frac{\gamma_j}{2\pi^2} \right)^{\lambda} \zeta(\alpha\lambda) \right) - 1 \right)^{1/2\lambda} \leq \exp\left(\frac{\zeta(\alpha\lambda)}{\lambda(2\pi^2)^{\lambda}} \sum_{j=1}^{d} \gamma_j^{\lambda} \right).$$

For any $\delta > 0$, choose λ to satisfy

$$-\frac{1}{2\lambda} = -\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} + \delta.$$

Then, we see that since $\lambda > \max(\frac{1}{s^*}, \frac{1}{\alpha})$,

$$C_{\infty,\lambda} = \lim_{d\to\infty} C_{d,\lambda} \leq \exp\left(\frac{\zeta(\alpha\lambda)}{\lambda(2\pi^2)^{\lambda}} \sum_{j=1}^{\infty} \gamma_j^{\lambda} \right) < \infty$$

which is independent of d and hence implies strong tractability. The rate of convergence is therefore

$$\mathcal{O}\left(n^{-\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} + \delta} \right)$$

for any $\delta > 0$. Taking δ arbitrarily small, we see that the ε-exponent of strong tractability lies in the range $(\frac{2}{\alpha}, \max(\frac{2}{s^*}, \frac{2}{\alpha})]$. □

Note that if $s^* \geq \alpha$ then the rate of convergence $\mathcal{O}\left(n^{-\alpha/2+\delta}\right)$ is achievable for arbitrarily small $\delta > 0$. Therefore, we may come arbitrarily close to the optimal rate of convergence $\mathcal{O}\left(n^{-\alpha/2}\right)$.

As was the case with Theorem 2.5.7, we can clearly drop the constraint on p in Theorem 2.5.10 with

Theorem 2.5.11 *Let $n = p^m$ be the power of a prime p and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$ a positive non-increasing sequence where* (2.20) *holds, then there exists a $\boldsymbol{z} \in \mathcal{Z}_{n,1}^d$ such that for all $\lambda \in (1/\alpha, 1]$*

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \overline{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda),$$

where

$$\overline{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) = n^{-1/\lambda} \left(\prod_{j=1}^{d} \left(1 + 4 \left(\frac{\gamma_j}{2\pi^2} \right)^{\lambda} \zeta(\alpha\lambda) \right) - 1 \right)^{1/\lambda}.$$

Remark 2.5.12 For the case where n being an arbitrary positive integer, the bound $\overline{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ may be replaced by $\widetilde{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ where

$$\widetilde{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) = n^{-1/\lambda} \left(\prod_{j=1}^{d} \left(1 + 2^{\kappa+1} \left(\frac{\gamma_j}{2\pi^2} \right)^{\lambda} \zeta(\alpha\lambda) \right) - 1 \right)^{1/\lambda}$$

and κ is the number of distinct prime factors of n. This bound will be used later in Chapter 5.

2.6 Construction of good lattice rules

We have established that if n is the power of a prime, then there exist generating vectors $\boldsymbol{z}$ which construct point sets in the Korobov space whose rate of convergence is arbitrarily close to the optimal rate of $\mathcal{O}\left(n^{-\alpha/2}\right)$.

All of the results presented thus far are existence results. In practice, we would like to be able to construct such generating vectors $\boldsymbol{z} \in \mathcal{Z}^d_{n,1}$ which achieve the optimal rate of convergence. (For simplicity we will refer to a generating vector or a lattice rule *achieving the optimal rate of convergence* $\mathcal{O}\left(n^{-\alpha/2}\right)$ if it achieves the rate $\mathcal{O}\left(n^{-\alpha/2+\delta}\right)$ for any $\delta > 0$.)

For $n = p^m$, the number of generating vectors $\boldsymbol{z} \in \mathcal{Z}^d_{p,m}$ is $\phi(p^m)^d = (p^{m-1}(p-1))^d$. Common problems will see the number of points $n = p^m$ in the thousands or higher and the dimension d in the hundreds, thousands, or higher. Therefore, a computer search of all possible generating vectors is infeasible. We must look for ways of reducing the search space. Below, we present two alternative ways of constructing a generating vector which achieves the optimal rate of convergence.

2.6.1 Korobov form

The Korobov form of a generating vector (not to be confused with the Korobov space) was first suggested by Korobov in [33, 34] and assumes that n is prime.

The generating vector has the form

$$\boldsymbol{z}_d(a) = (1, a, a^2, \ldots, a^{d-1}) \pmod{n}$$

for some $a \in \{1, 2, \ldots, n-1\}$. Using an averaging argument and the Jensen's inequality, it can be shown [61] that there exists an $a \in \{1, 2, \ldots, n-1\}$, such that for all $\lambda \in (1/\alpha, 1]$, the generating vector $\boldsymbol{z}(a) = (1, a, a^2, \ldots, a^{d-1})$ (mod n) has a worst-case error bounded by

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda), \tag{2.43}$$

where

$$\widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) = (n-1)^{-1/\lambda} d^{1/\lambda} \prod_{j=1}^{d} \left(1 + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(\alpha\lambda)\right)^{1/\lambda}$$

Note that (2.43) can be re-written as

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq C_{\mathrm{kor},d,\lambda} d^{1/(2\lambda)} n^{-1/(2\lambda)},$$

where

$$\begin{aligned} C_{\mathrm{kor},d,\lambda} &= 2^{1/(2\lambda)} \prod_{j=1}^{d} \left(1 + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(\alpha\lambda)\right)^{1/(2\lambda)} \\ &\leq 2^{1/(2\lambda)} \exp\left(\frac{\zeta(\alpha\lambda)}{\lambda(2\pi^2)^{\lambda}} \sum_{j=1}^{\infty} \gamma_j^{\lambda}\right) = C_{\mathrm{kor},\infty,\lambda} < \infty. \end{aligned}$$

If, as in Section 2.5.3, we choose λ to satisfy

$$-\frac{1}{2\lambda} = -\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} + \delta$$

for any $\delta > 0$, then we may bound the worst-case error by

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq C_{\mathrm{kor},\infty}(\delta) d^{\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} - \delta} n^{-\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} + \delta}$$

where s^* is defined as in (2.40) and $C_{\mathrm{kor},\infty}(\delta) = C_{\mathrm{kor},\infty,\lambda}$ for the choice of λ.

We see that it is possible to achieve the optimal rate of convergence with polynomial dependence on d. Also, it is clear that we have tractability but not

strong tractability; the quantity $n(\varepsilon, d; K_{\mathrm{per},d,\alpha,\boldsymbol{\gamma}})$ depends at most linearly on the d.

Since the search space is reduced to $n-1$ possible choices for a, it is feasible to search through all possible choices and locate one which satisfies this bound. By the theory above, we know at least such a one exists.

While it is possible to achieve the optimal rate of convergence with generating vectors of the Korobov form, the method does have certain weaknesses. Firstly, the method considers only a very small subset of generating vectors. Secondly, the dependence of the upperbound on the worst-case error (2.43) on the variable d is not ideal. Thirdly, the number of points n must be prime. There are results (see Wang et al [61]) for constructing rules of the Korobov form with the number of points being a product of *distinct* primes. However, in this case the optimal rate of convergence is not achieved. Finally, the generating vector $\boldsymbol{z}_d(a)$ is good for only one value of d, that is, it is not extensible in dimension. We will see in Chapter 6 that this final problem can be overcome.

In the meantime, we describe another method of constructing the generating vector which has proven to be of great practical value.

2.6.2 Component-by-component algorithm

The component-by-component (CBC) algorithm was developed by, among others, Sloan, Reztsov, Joe, Kuo and Dick (see [54, 52, 53, 8, 10]). As the name suggests, the central idea behind the algorithm is to construct the generating vector $\boldsymbol{z}$ one component at a time. For an $n = p^m$-point lattice rule, at each of the d dimensions, there is a choice between $\phi(p^m)$ different components. Therefore, the size of the search space is $d\phi(p^m)$, rather than $\phi(p^m)^d$.

In simple terms, given a generating vector $\boldsymbol{z}_d^* = (z_1^*, z_2^*, \ldots, z_d^*)$, the CBC chooses the component z_{d+1}^* which minimises the quantity

$$e_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}^*, z_{d+1}))$$

over all possible choices $z_{d+1} \in \mathcal{Z}_{p,m}$. It is simple to see that all choices to

z_1 have equal worst-case error if z_1 is co-prime with $n = p^m$, so we will by convention take $z_1 = 1$. The CBC algorithm is stated formally in Algorithm 1.

Algorithm 1 CBC algorithm

Require: Let $n = p^m$ be the power of a prime p, $\alpha > 1$, $d_{\max}$ some integer

1: Set $z_1^* = 1$
2: **for** $d = 1$ to $d_{\max} - 1$ **do**
3: Find $z_{d+1}^* \in \mathcal{Z}_{p,m}$ which minimises $e_{\text{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))$
4: Set $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$
5: **end for**

We now present a proof that for $n = p^m$ being a power of a prime p, the CBC algorithm can achieve the optimal rate of convergence. The proof is similar to that of [35] and [8].

Theorem 2.6.1 *Let $n = p^m$ be a power of a prime p and $d_{\max}$ be some integer. Then the CBC algorithm, as described above in Algorithm 1, constructs a generating vector $\boldsymbol{z}_d^*$ such that for all $\lambda \in (1/\alpha, 1]$*

$$e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \le \overline{M}^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $d = 1, 2, \ldots, d_{\max}$.

Proof. We first show this for the case where $\lambda = 1$. That is, we show that

$$e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \le \overline{M}^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}} = \frac{1}{n}\left(\prod_{j=1}^{d}\left(1 + 4\frac{\gamma_j}{2\pi^2}\zeta(\alpha)\right) - 1\right).$$

So as to make the later use of the Jensen's inequality clear, we will sometimes leave uncancelled terms in fractions. We now prove the CBC algorithm by induction. Beginning with the $d = 1$ and $z_1^* = 1$, we see from (2.30) and (2.32)

that

$$e^2_{\mathrm{per},p^m,1,\alpha,\gamma_1}(z_1^*) = -1 + \frac{1}{p^m}\sum_{k=0}^{p^m-1}\left(1 + \frac{\gamma_j}{2\pi^2}\sum_{h\in\mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} kh/n}}{|h|^\alpha}\right)$$
$$= \sum_{h\in\mathbb{Z}}{}' \frac{\gamma_j}{2\pi^2}\frac{1}{|h|^\alpha}\frac{1}{p^m}\sum_{k=0}^{p^m-1}\mathrm{e}^{2\pi\mathtt{i}kh/p^m}$$
$$\leq \frac{2}{p^m}\frac{\gamma_j}{2\pi^2}\zeta(\alpha) \leq \overline{M}^2_{\mathrm{per},p^m,1,\alpha,\gamma_1}.$$

Now assume for some integer d that

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \leq \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}. \tag{2.44}$$

We will show that if we choose z_{d+1}^* to minimise $e_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))$, then

$$e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}^*)) \leq \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}.$$

We begin by defining the quantity

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) = e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1})) - e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*), \tag{2.45}$$

and showing that

$$\frac{1}{\phi(p^m)}\sum_{z_{d+1}\in\mathcal{Z}_{p,m}} \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \leq \overline{\theta}_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}$$

where

$$\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}} = \frac{4}{p^m}\frac{\gamma_{d+1}}{2\pi^2}\zeta(\alpha)\prod_{j=1}^{d}\left(1 + 2\frac{\gamma_j}{2\pi^2}\zeta(\alpha)\right).$$

From (2.30) we see that

$$\begin{aligned}
&\frac{1}{\phi(p^m)} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \\
&= \left| \frac{1}{p^m} \sum_{k=0}^{p^m-1} \prod_{j=1}^{d} \left(1 + \frac{\gamma_j}{2\pi^2} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z_j^*/p^m}}{|h|^\alpha} \right) \times \right. \\
&\qquad \left. \left[\frac{1}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \sum_{z_{s+1} \in \mathcal{Z}_{p,m}} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z_{d+1}/p^m}}{|h|^\alpha} \right] \right| \\
&\le \frac{1}{p^m} \sum_{k=0}^{p^m-1} \prod_{j=1}^{d} \left| 1 + 2\frac{\gamma_j}{2\pi^2} \sum_{h=1}^{\infty} \frac{\cos(2\pi k h z_j^*/p^m)}{|h^\alpha|} \right| \times \\
&\qquad \left| \frac{1}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z_{d+1}/p^m}}{|h|^\alpha} \right| \\
&\le \frac{1}{p^m} \sum_{k=0}^{p^m-1} \prod_{j=1}^{d} \left(1 + 2\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right) \left| \frac{1}{\phi(p^m)} \frac{\gamma_{d+1}}{2\pi^2} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z_{d+1}/p^m}}{|h|^\alpha} \right| \\
&\le \frac{4}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \zeta(\alpha) \prod_{j=1}^{d} \left(1 + 2\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right)
\end{aligned}$$

where the final line uses the result in [36, Lemma 2.1 and Lemma 2.3] which says that for m any integer

$$\sum_{k=0}^{p^m-1} \left| \frac{1}{\phi(p^m)} \sum_{z \in \mathcal{Z}_{p,m}} \sum_{h \in \mathbb{Z}}{}' \frac{\mathrm{e}^{2\pi \mathtt{i} k h z/p^m}}{|h|^\alpha} \right| \le 4\zeta(\alpha). \tag{2.46}$$

This tells us that for any given $\boldsymbol{z}_d^*$, there must exist a $z_{d+1}^* \in \mathcal{Z}_{p,m}$ such that

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \le \frac{4}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \zeta(\alpha) \prod_{j=1}^{d} \left(1 + 2\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right) \tag{2.47}$$

Putting the inductive assumption (2.44) together with (2.47) we see that

$$\begin{aligned}
&e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \\
&\le \frac{1}{p^m} \left(\prod_{j=1}^{d} \left(1 + 4\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right) - 1 \right) + \frac{4}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \zeta(\alpha) \prod_{j=1}^{d} \left(1 + 2\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right) \\
&\le \frac{1}{p^m} \left(\prod_{j=1}^{d+1} \left(1 + 4\frac{\gamma_j}{2\pi^2} \zeta(\alpha) \right) - 1 \right).
\end{aligned}$$

We have now shown the special case of the theorem where $\lambda = 1$. We will now prove the more general case where $\lambda \in (1/\alpha, 1]$. Before we begin, recall the result in (2.42) which says that for all $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$ and $\lambda \in (1/\alpha, 1]$

$$e^2_{\text{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq [e^2_{\text{per},p^m,d,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}(\boldsymbol{z})]^{1/\lambda}.$$

We first derive a similar result for $\theta_{\text{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$. Note that by (2.31), we can also write $\theta_{\text{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$ in the form

$$\begin{aligned}
&\theta_{\text{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \\
&= \sum_{\substack{(\boldsymbol{h},h_{d+1})\in\mathbb{Z}^{d+1}\setminus\{\boldsymbol{0}\} \\ (\boldsymbol{h},h_{s+1})\cdot(\boldsymbol{z}_d^*,z_{d+1})\equiv 0 \pmod{p^m}}} \frac{1}{r_\alpha((\boldsymbol{h},h_{d+1}),\boldsymbol{\gamma})} - \sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^d\setminus\{\boldsymbol{0}\} \\ \boldsymbol{h}\cdot\boldsymbol{z}_d^*\equiv 0 \pmod{p^m}}} \frac{1}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})} \\
&= \sum_{\substack{(\boldsymbol{h},h_{d+1})\in\mathbb{Z}^{d+1},h_{d+1}\neq 0 \\ (\boldsymbol{h},h_{d+1})\cdot(\boldsymbol{z}_d^*,z_{d+1})\equiv 0 \pmod{p^m}}} \frac{1}{r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})}. \qquad (2.48)
\end{aligned}$$

Note that each term in the expression in (2.48) is positive. This allows us to apply the Jensen's inequality to (2.48), which, recalling (2.42), allows us to write

$$\begin{aligned}
\theta_{\text{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) &\leq \left(\sum_{\substack{(\boldsymbol{h},h_{d+1})\in\mathbb{Z}^{d+1},h_{d+1}\neq 0 \\ (\boldsymbol{h},h_{d+1})\cdot(\boldsymbol{z}_d^*,z_{d+1})\equiv 0 \pmod{p^m}}} \frac{1}{[r_\alpha(\boldsymbol{h},\boldsymbol{\gamma})]^\lambda} \right)^{1/\lambda} \\
&= \left(\sum_{\substack{(\boldsymbol{h},h_{d+1})\in\mathbb{Z}^{d+1},h_{d+1}\neq 0 \\ (\boldsymbol{h},h_{d+1})\cdot(\boldsymbol{z}_d^*,z_{d+1})\equiv 0 \pmod{p^m}}} \frac{1}{r_{\alpha\lambda}(\boldsymbol{h},2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda)} \right)^{1/\lambda} \\
&= [\theta_{\text{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}(\boldsymbol{z}_d^*, z_{d+1})]^{1/\lambda}. \qquad (2.49)
\end{aligned}$$

We are now ready to prove the main result using induction. It is clear from above that when $d = 1$ and $z_1^* = 1$, for all $\lambda \in (1/\alpha, 1]$

$$e^2_{\text{per},p^m,1,\alpha,\gamma_1}(z_1^*) \leq \overline{M}^2_{\text{per},p^m,1,\alpha,\gamma_1}(\lambda).$$

We now assume for some integer d that

$$e^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \leq \overline{M}^2_{\text{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

In a similar vein to the first part of the proof we see that if z_{d+1}^* is chosen to minimise $e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$ for given $\boldsymbol{z}^*$, then by (2.49) z_{d+1}^* must satisfy

$$\begin{aligned}\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) &\le [\theta_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}(\boldsymbol{z}_d^*, z_{d+1}^*)]^{1/\lambda} \\ &\le [\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}]^{1/\lambda}\end{aligned}$$

Putting this together with the inductive assumption, we see that

$$\begin{aligned}e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) &= e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) + \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \\ &\le \overline{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) + [\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}]^{1/\lambda} \\ &\le \frac{1}{p^{m/\lambda}}\left(\prod_{j=1}^{d}\left(1+4\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\right)-1\right) \\ &\quad + \frac{4}{p^{m/\lambda}}\left(\frac{\gamma_{d+1}}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\prod_{j=1}^{d}\left(1+2\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\right) \\ &\le \frac{1}{p^{m/\lambda}}\left(\prod_{j=1}^{d+1}\left(1+4\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\right)-1\right),\end{aligned}$$

where the final inequality follows by another application of the Jensen's inequality. Therefore, for $n = p^m$, the power of a prime p, we see that a vector $\boldsymbol{z}^*$ may be constructed for arbitrary dimension d such that for all $\lambda \in (1/\alpha, 1]$

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \le n^{-1/\lambda}\left(\prod_{j=1}^{d}\left(1+4\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\right)-1\right)^{1/\lambda}.$$

□

We can see that if the vector $\boldsymbol{z}$ is constructed with the CBC algorithm, then for any $\lambda \in (1/\alpha, 1]$ the worst-case error can be written in the form

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le C_{\mathrm{cbc},d,\lambda}\, n^{-1/2\lambda},$$

where

$$\begin{aligned}C_{\mathrm{cbc},d,\lambda} &= \prod_{j=1}^{d}\left(1+4\left(\frac{\gamma_j}{2\pi^2}\right)^\lambda\zeta(\alpha\lambda)\right)^{1/2\lambda} \\ &\le \exp\left(\frac{2\zeta(\alpha\lambda)}{\lambda(2\pi^2)^\lambda}\sum_{j=1}^{\infty}\gamma_j^\lambda\right) = C_{\mathrm{cbc},\infty,\lambda} < \infty.\end{aligned}$$

If, as in Section 2.5.3, we choose λ to satisfy

$$-\frac{1}{2\lambda} = -\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})} + \delta$$

for any $\delta > 0$, then we may bound the worst-case error by

$$e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq C_{\mathrm{cbc},\infty}(\delta) n^{-\frac{1}{\max(\frac{2}{s^*}, \frac{2}{\alpha})}+\delta}$$

where s^* is defined as in (2.40) and $C_{\mathrm{cbc},\infty}(\delta) = C_{\mathrm{cbc},\infty,\lambda}$ for the choice of λ. Taking δ arbitrarily small, we see that the ε-exponent of strong tractability lies in the range $[\frac{2}{\alpha}, \max(\frac{2}{s^*}, \frac{2}{\alpha})]$.

2.6.3 Fast component-by-component construction

The cost of constructing the n-point lattice rule for d dimensions is $\mathcal{O}(n^2d^2)$ operations which can be reduced to $\mathcal{O}(n^2d)$ operations by storing the product terms during the search. This storage requires $\mathcal{O}(n)$ storage. This cost corresponds to a matrix-vector multiplication which costs $\mathcal{O}(n^2)$ which must be performed d times. The matrix in the matrix-vector multiplication is based upon the matrix

$$[kz \pmod n]_{\substack{1\leq k\leq n \\ 1\leq z\leq n-1}}.$$

It was pointed out by Nuyens and Cools [45, 47, 46], that the $n \times n$ matrix in this multiplication contains the same n entries in each column. Moreover, they showed a way to permute the rows and columns of this matrix to turn it into a circulant matrix.

For example, taking $n = 5$, (discarding the trivial column where $k = n$) we obtain a matrix which, with a permutation of its columns and then its rows, gives us a circulant matrix:

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 1 & 3 \\ 3 & 1 & 4 & 2 \\ 4 & 3 & 2 & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 2 & 4 & 3 \\ 2 & 4 & 3 & 1 \\ 3 & 1 & 2 & 4 \\ 4 & 3 & 1 & 2 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 2 & 4 & 3 \\ 3 & 1 & 2 & 4 \\ 4 & 3 & 1 & 2 \\ 2 & 4 & 3 & 1 \end{bmatrix}.$$

For an $n \times n$ circulant matrix C_n with first column $\boldsymbol{c}$, the matrix-vector multiplication $C_n\boldsymbol{x}$ can be performed in $\mathcal{O}(n \log n)$ operations by

$$C_n\boldsymbol{x} = \text{IFFT}(\text{FFT}(\boldsymbol{c}) \ .* \ \text{FFT}(\boldsymbol{x})),$$

where we adopt the MATLAB notation $.*$ for a componentwise multiplication and FFT and IFFT correspond to the Fast Fourier Transform and Inverse Fast Fourier Transform respectively.

The CBC algorithm which exploits this property is known as the *fast CBC* algorithm and has total cost of $\mathcal{O}(n \log(n)\, d)$ operations. This allows the practical computation of good generating vectors for problems of a realistic scale.

2.7 Applications of multivariate integration to financial mathematics

There is tremendous practical interest in high-dimensional multivariate integration from the financial mathematics community. We shall see shortly how many problems of mathematical finance can be solved using MC or QMC techniques. Indeed, we should remember that much of the interest in QMC techniques has been spurred on by the work of Paskov and Traub [49], who showed that QMC techniques performed much better than MC for the collateralised mortgage-backed obligations problem.

In this thesis, we will focus on the Asian option problem. This is a different style of problem to that considered by Paskov and Traub. We will see that QMC methods can make a remarkable improvement upon MC methods. Before we delve into the details of the problem, we provide a short introduction on the nature of these problems. Please note that this introduction is by no means comprehensive. For a deeper look at the problems of financial mathematics see Hull [31]; and for a more specific examination of the use of MC and QMC techniques in finance problems, see Glasserman [17].

2.7.1 Basic finance problems

Around the world there are many exchanges where the trading of different assets takes place. Tradable assets include government bonds, shares in companies, different currencies and commodities such as gold, crude oil, natural gas, wheat, barley and pork bellies. Additionally, there is an exponentially growing *derivatives* market. These are markets where the products traded are derived from some underlying traded asset.

For a simple example as to why such a market is attractive, consider an airline. Aviation fuel is obviously a very large component of their costs. When the price of fuel rises dramatically, the profitability of the business may suffer. Therefore, the airline might buy an *option* on aviation fuel. This is the right, but not the obligation to buy fuel at some pre-determined price. A typical contract might be to buy 1000 units of fuel at, say, US$100 per unit in one years time. If the market price of the fuel in one years time is US$80, then it does not make sense to exercise the option. However, if the market price of the fuel in one years time is US$120, then the option will be exercised. In the former case, when the option was not exercised, the *payoff* is said to be zero. In the latter case, the payoff would be US$20.

The problem for the financial mathematician is to calculate a fair price now for such an option, or indeed any such derivative.

2.7.2 Problem formulation

We will formulate the problems of financial mathematics using *arbitrage-free pricing*. Put simply, this means that prices in the market are at such a level that participants in the market cannot make risk-free profits.

As a simple example of a market, consider a game where an unbiased coin is tossed regularly. Participants can pay an entry fee to the game. The participants are paid $1 if a "heads" is thrown and receive nothing if a "tails" is thrown. The fair value of entry to this game is clearly 50 cents. If the price

in the marketplace were anything different, then a simple arbitrage strategy would ensure risk-free profits.

The outcomes of a stock market are, of course, more complicated than that of a simple coin-tossing exercise. However, the principle remains the same. The fair value of a derivative is the *present value* of the expected value of the payoff. The expected value is taken with respect to some risk-neutral probability measure. The present value part simply discounts the future payoff cashflows back to their current value. Put simply, $\$x$ received T years in the future has a present value of $\$x\mathrm{e}^{-rT}$ in the present, where r is the continuously compounded risk-free interest rate, whose value is known from the market price of traded government bonds.

There are several different models which are used to model stock price movements. One of the more popular models is the famous *Black-Scholes* model, developed by Black and Scholes [3] and Merton [40]. Under this model, the price of a stock is assumed to follow the stochastic differential equation (SDE)

$$\frac{\mathrm{d}S(t)}{S(t)} = r\,\mathrm{d}t + \sigma\,\mathrm{d}W(t) \tag{2.50}$$

where W is a standard Brownian motion and σ is a parameter representing the volatility of the stock price. The value of σ is usually measured from market data (see [31]).

The SDE in (2.50) has solution

$$S(t) = S_0 \exp\left((r - \tfrac{1}{2}\sigma^2)t + \sigma W(t)\right) \tag{2.51}$$

where S_0 is the stock price at $t = 0$, which we will assume is known.

Remark 2.7.1 In this thesis we shall make the simplifying assumptions that the risk-free rate r and volatility σ are fixed over the life of the product. This is typically not true in practice. The Black-Scholes model can be generalised so that r and σ may vary, either deterministically, or stochastically (see Heston [21]). We will also assume that there are no dividends paid on any stocks.

The random variable $W(t)$ in (2.51) is normally distributed with mean 0 and variance t. We may therefore replace $W(t)$ with $\sqrt{t}Z$, where Z is a standard normal random variable. We can see that $\log S(t)$ is normally distributed. Therefore, the stock price $S(t)$ is said to be log-normally distributed.

The payoff of an option *exercisable* at time T, where the payoff is dependent only on the final price $S(T)$, is known as a *European* option. A common example is the European *call* option with strike price K, whose payoff is given by

$$g(S(T)) = (S(T) - K)^+ \tag{2.52}$$

where $(x)^+$ is equal to the greater of x and 0. If the option is exercisable *before* the time T, then it is known as an *American* option.

We shall be interested in another type of option known as an *Asian* option. This is an option which is dependent on the whole trajectory of the share price $S(t)$ for $t \in [0, T]$, not just the final price $S(T)$. For example, an (arithmetic) Asian call option is often defined to be a derivative with payoff

$$g(S(t) : t \in [0, T]) = \left(\frac{1}{T} \int_0^T S(t)\, \mathrm{d}t - K \right)^+ . \tag{2.53}$$

The arbitrage-free price of such a derivative is given by

$$\mathbb{E}\left[\mathrm{e}^{-rT} g(S(t) : t \in [0, T]) \right] \tag{2.54}$$

where the expectation is taken with respect to the log-normal density of $S(t)$. That is, we integrate the payoff over all possible paths $S(t)$ and discount the value to find the arbitrage-free price. In the case of the European call option in (2.52), this has a closed-form solution

$$\mathbb{E}[\mathrm{e}^{-rT}(S(T) - K)^+] = S_0 \Phi\left(d_1\right) - \mathrm{e}^{-rT} K \Phi\left(d_2\right),$$

where

$$d_{1,2} = \frac{\log(S_0/K) + (r \pm \frac{1}{2}\sigma^2)/T}{\sigma\sqrt{T}}$$

and Φ is the cumulative normal distribution, defined by

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \mathrm{e}^{-\frac{1}{2}t^2}\, \mathrm{d}t.$$

However, this is a special case. In general, the expression (2.54) will not have a closed-form solution.

The space of all Brownian motion paths is an infinite-dimensional space. We must therefore reduce the dimensionality of the problem.

2.7.3 Application of MC and QMC

In the examples considered in this thesis, we will approximate the continuous solution of the SDE (2.51) with d equally-spaced time discretisations at times $t_j = j\Delta t$ for $j = 0, 1, \ldots, d$ where $\Delta t = T/d$, which gives us

$$S(t_j) = S_0 \exp\left((r - \tfrac{1}{2}\sigma^2)t_j + \sigma W(t_j)\right), \quad j = 1, \ldots, d. \tag{2.55}$$

Our method of discretising the stock prices is therefore simply discretising the Brownian motion W at the times t_j for $j = 1, \ldots, d$.

Remark 2.7.2 The use of the discretisation does introduce bias into the problem. However, this bias is not completely undesirable, since most seemingly continuous problems in the real world are in fact discrete. For example, stock prices are generally rounded to the nearest cent, and times to the nearest second. An Asian problem like the one described in (2.53) may in fact monitored daily, or perhaps less frequently. We shall therefore generally assume that the value of d is set to reflect the "natural" level of discretisation in the market.

Let us take $\boldsymbol{u} = (W(t_1), \ldots, W(t_d))^T$ to be the vector with the value of the Brownian motion at each time discretisation. The vector $\boldsymbol{u}$ is therefore a multivariate normal distribution with zero mean and symmetric positive-definite covariance $\Sigma = (\Sigma_{i,j})_{i,j=1}^d$ matrix given by

$$\Sigma_{i,j} = \min(t_i, t_j). \tag{2.56}$$

The Asian option with payoff given in (2.53) is therefore the continuous analogue of the discretised Asian option with payoff

$$G(\boldsymbol{u}) = g(S(t_1), \ldots, S(t_d)) = \left(\frac{1}{d}\sum_{j=1}^{d} S(t_j) - K\right)^+, \tag{2.57}$$

where $S(t_j)$ is formulated as in (2.55). When we now refer to an "Asian option", we will always be referring to this discretised version. Using (2.54), we see that the arbitrage-free price of such a derivative is

$$C = \int_{\mathbb{R}^d} \frac{\mathrm{e}^{-rT}}{(\sqrt{2\pi})^d \sqrt{\det \Sigma}} G(\boldsymbol{u}) \exp\left(-\tfrac{1}{2}\boldsymbol{u}^T \Sigma^{-1} \boldsymbol{u}\right) \mathrm{d}\boldsymbol{u}. \tag{2.58}$$

We now attempt to find an approximate solution to (2.58) using MC and QMC techniques. The usual form to take such a problem (2.1) is an integral over the unit cube. We therefore begin by mapping (2.58) to the unit cube.

We begin by making the substitution $\boldsymbol{u} = A\boldsymbol{z}$, where A is any matrix such that $AA^T = \Sigma$. This allows us to write

$$\begin{aligned} C &= \int_{\mathbb{R}^d} \frac{\mathrm{e}^{-rT}}{(\sqrt{2\pi})^d \sqrt{\det \Sigma}} G(\boldsymbol{u}) \exp\left(-\tfrac{1}{2}\boldsymbol{u}^T \Sigma^{-1} \boldsymbol{u}\right) \mathrm{d}\boldsymbol{u} \\ &= \int_{\mathbb{R}^d} \frac{\mathrm{e}^{-rT}}{(\sqrt{2\pi})^d} G(A\boldsymbol{z}) \exp\left(-\tfrac{1}{2}\boldsymbol{z}^T \boldsymbol{z}\right) \mathrm{d}\boldsymbol{z} \\ &= \int_{[0,1]^d} \mathrm{e}^{-rT} G(A\Phi^{-1}(\boldsymbol{x})) \, \mathrm{d}\boldsymbol{x} \end{aligned}$$

where $\Phi^{-1}(\boldsymbol{x}) = (\Phi^{-1}(x_1), \ldots, \Phi^{-1}(x_d))$ is a vector of componentwise inverse cumulative density functions.

We can now write the arbitrage-free value of the Asian option in the form of the integral problem (2.1), that is

$$C = \int_{[0,1]^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}, \quad \text{where } f(\boldsymbol{x}) = \mathrm{e}^{-rT} G(A\Phi^{-1}(\boldsymbol{x})). \tag{2.59}$$

2.7.4 Covariance matrices

In the section above, we needed to find a matrix A such that $AA^T = \Sigma$ for $t_i = i\Delta t$, where Σ is the covariance matrix. The choice of the matrix A will play an important role in the performance of the lattice rules.

The vector $\boldsymbol{u} = (W(t_1), \ldots, W(t_d))^T$ is constructed by $\boldsymbol{u} = A\boldsymbol{z}$, where $\boldsymbol{z} = (z_1, \ldots, z_d)$ is a vector of i.i.d. standard normal variables. The choice of A will determine how the vector $\boldsymbol{y}$ and hence the path $S(t)$ is constructed.

Standard construction

There are three common choices for this matrix A. The first, usually referred to as the *standard construction*, is to choose the Cholesky factor of Σ. For this particular matrix Σ, the Cholesky factor has the simple form

$$A = \sqrt{\Delta t} \begin{pmatrix} 1 & 0 & \dots & 0 \\ 1 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix}. \tag{2.60}$$

This choice of A corresponds to sequentially generating the Brownian path, one increment after another. It is clear that taking $W(t_0) = 0$, the path is constructed by

$$W(t_j) = W(t_{j-1}) + \sqrt{\Delta t} z_j \quad \text{for } j = 1, \dots, d.$$

The use of the standard construction is attractive from a computation perspective since the matrix-vector multiplication $A\boldsymbol{z}$ is, in effect, just a cumulative sum of the components of the vector $\boldsymbol{z}$.

Brownian bridge

The *Brownian bridge construction* differs from the standard construction in that rather than constructing the increments sequentially, the coarse outline of the path of $W(t_j)$ for $j = 1, \dots, d$ is constructed and then progressively refined.

It is easiest to see this for the case where d is some power of 2. We first construct the endpoint $W(T)$, then the midpoint $W(T/2)$, then the midpoints of each segment $W(T/4)$ and $W(3T/4)$ and so on, each time finding the new midpoint of each segment.

Formally, the path $W(t_j)$ for $j = 1, \ldots, d$ is constructed by

$$\begin{aligned}
W(0) &= 0 \\
W(T) &= \sqrt{T} z_1 \\
W(T/2) &= \frac{W(0) + W(T)}{2} + \sqrt{\frac{T}{4}} z_2 \\
W(T/4) &= \frac{W(0) + W(T/2)}{2} + \sqrt{\frac{T}{8}} z_3 \\
W(T/4) &= \frac{W(T/2) + W(T)}{2} + \sqrt{\frac{T}{8}} z_4 \\
&\vdots \\
W((d-1)T/d) &= \frac{W((d-2)T/d) + W(T)}{2} + \sqrt{\frac{T}{2d}} z_d.
\end{aligned}$$

Although this can be formulated into a matrix A, in practice it is more efficient to use the structure above to calculate $W(t_j)$ for $j = 1, \ldots, d$.

The Brownian bridge construction has the effect of placing more importance on the earlier variables than the later variables. To see this, for d being some power of 2, consider the paths of $W(t_j)$ for $j = 1, \ldots, d$, if the variables $z_{d/2+1}, \ldots, z_d$ were "lost". Under the standard construction, the path would be unknown past $W(t_{d/2})$. However, under the Brownian bridge construction, the general shape of the path would be clear, with every second point "smoothed out".

The placement of greater importance on the leading variables is an attractive feature for lattice rules. It allows us to focus on getting good projections in the smaller number of important variables. This is the purpose of the weights which were described in Section 2.4.1.

Principal components analysis construction

We have seen that the Brownian bridge construction places greater emphasis on the earlier variables, which is attractive for our weighted lattice rules. It

is therefore natural to seek a construction which maximises the importance of the leading variables. The answer to such a problem lies in the *principal components analysis construction* (PCA).

If we re-write the matrix vector multiplication $\boldsymbol{u} = A\boldsymbol{z}$ as

$$\boldsymbol{u} = \boldsymbol{a}_1 z_1 + \boldsymbol{a}_2 z_2 + \cdots + \boldsymbol{a}_d z_d$$

where $\boldsymbol{a}_j$ is the j-th column of A, we would like to find the choice of $\boldsymbol{a}_j$ for $j = 1, \ldots, d$ which minimises the approximation error

$$\mathbb{E}\left[\|\boldsymbol{u} - \sum_{i=1}^{j} \boldsymbol{a}_i z_i\|^2\right].$$

By Rayleigh's principle, it can be seen that the minimum is achieved when for $j = 1, \ldots, d$ we take

$$\boldsymbol{a}_j = \sqrt{\lambda_j}\boldsymbol{v}_j \tag{2.61}$$

where $\lambda_1 > \lambda_2 > \cdots > \lambda_d > 0$ are the eigenvalues of Σ and the $\boldsymbol{v}_j$'s are the corresponding unit-length eigenvectors.

It has been noted by Glasserman [17] that a weakness of the PCA method is that the matrix-vector multiplication requires $\mathcal{O}(d^2)$ operations, whereas the structure of the standard and Brownian bridge constructions mean only $\mathcal{O}(d)$ operations are needed to construct the discretised Brownian motion path. However, recent work by Giles [16] suggests the use of an FFT to reduce this cost to $\mathcal{O}(d \log d)$.

2.8 Difficulty applying lattice rules to finance problems

In this chapter we have given a very brief overview of the theory of multivariate integration, and more specifically lattice rules, as well as a description of the types of integration problems encountered in mathematical finance. It is natural to now seek to apply the lattice rules technology to the finance problems.

However, there are several issues and problems in trying to apply the lattice rules to these problems. Some of these problems are theoretical, while some are practical.

The first problem is a theoretical one. In Section 2.5, we analysed lattice rules (usually randomly-shifted) in weighted Korobov and weighted Sobolev spaces. However, the integrands in the finance problems, for example the one presented in (2.59), do not lie in the weighted Sobolev space.

A second problem concerns the practical application of lattice rules. A practitioner would ideally like to use only as many points (and hence function evaluations) as required to get an answer within the desired level of accuracy.

For QMC point sets based on open-ended sequences, this is not a problem. However, our theory assumes that we will always evaluate all n-points in each lattice rule. If n is too large, then the practitioner will have wasted computational time. On the other hand, if n is not sufficiently large to achieve the desired error bound, then the process must begin again from scratch, because the lattice rules constructed by the Korobov or CBC algorithms are dependent upon n. It would be advantageous to be able to construct lattice rules which are *good* for a range of values of n.

The remainder of the thesis will deal with attempting to solve these two problems.

Chapter 3

Multivariate integration for a class of unbounded analytic functions

This chapter of the thesis is based on work which appeared in [65]. Some of the results have been generalised for the thesis.

We have seen in Section 2.7 that many finance problems such as (2.58) are formulated as integrals of the form

$$I_{\rho_d}(g) = \int_{\mathbb{R}^d} g(\boldsymbol{u})\rho_d(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} \tag{3.1}$$

where

$$\rho_d(\boldsymbol{u}) = \frac{1}{(\sqrt{2\pi})^d\sqrt{\det\Sigma}}\exp\left(-\tfrac{1}{2}\boldsymbol{u}^T\Sigma^{-1}\boldsymbol{u}\right)$$

for some payoff function g and some covariance matrix Σ. Using a matrix factorisation of the form $AA^T = \Sigma$ and mapping this back to the unit cube by means of the inverse cumulative normal density Φ_d^{-1}, where $\Phi_d^{-1}(\boldsymbol{x}) = (\Phi^{-1}(x_1),\ldots,\Phi^{-1}(x_d))^T$, the derivative pricing problem corresponds to the integral

$$I_{\rho_d}(g) = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = I_d(f), \quad \text{where } f(\boldsymbol{x}) = g(A\Phi_d^{-1}(\boldsymbol{x})). \tag{3.2}$$

The transformation described above almost inevitably leads to an integration problem over the unit cube for which the integrand blows up near the boundary. Typical functions g arising in mathematical finance are exponential in character (see for example Hull [31]), thus we introduce a function class that allows functions g that are exponential. In this introduction, however, as an illustration we will take g to be linear and d to be 1, that is

$$g(u) = a + bu, \quad u \in \mathbb{R},$$

for some a, $b \in \mathbb{R}$, so that (taking $A = 1$) the final integral (3.2) becomes

$$I_\rho(g) = \int_0^1 \left(a + b\,\Phi^{-1}(x)\right)\,\mathrm{d}x. \tag{3.3}$$

Note, for simplicity, we will write ρ_1 simply as ρ.

The graph of Φ^{-1}, shown in Figure 3.1, shows the essential problem: that unless g itself is bounded, the transformation process induces unbounded (but weakly singular) behaviour on the boundary of $[0, 1]$.

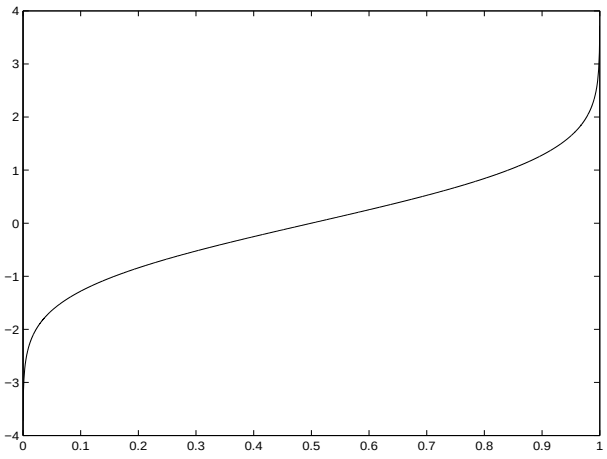

Figure 3.1: Graph of $\Phi^{-1}(x)$

MC methods have no problem with an integral such as (3.3), or in higher dimensions the more general (3.2), because MC methods work for any $f \in L_2([0, 1]^d)$ with moderate variance. QMC methods, on the other hand, have a serious difficulty with unbounded integrands, in that the error may be infinite if any point $\boldsymbol{t}_k$ is on the boundary.

Owen [48] addresses the problem of unbounded integrands in the context of low-discrepancy QMC methods by studying, and if necessary modifying, the location of integration points that lie close to the boundary.

Our approach in this chapter is different. We tackle the problem of unbounded or irregular integrands f by using *randomly-shifted* rank-1 lattice rules – that is to say, the shift $\boldsymbol{\Delta}$ in (2.29), instead of being a fixed vector in $[0,1]^d$, is now chosen randomly from a uniform distribution on $[0,1]^d$. The first advantage is that the unbounded integrands arising from the transformation process no longer cause concern. There is also a second advantage (first pointed out by Cranley and Patterson [5], see also [32, 52]) that the random nature of the shift allows (just as for MC methods) the easy computation of a probabilistic error estimate.

We study a completely different reproducing kernel Hilbert space $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$, but one which is again a tensor-product space with weights $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$. A key feature which distinguishes our space $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ from other spaces studied earlier is that typical functions in our space are unbounded near the boundary. The functions in our space $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ are of the form

$$f(\boldsymbol{x}) = g(\Phi_d^{-1}(\boldsymbol{x})),$$

where $g(\boldsymbol{u})$ is some function on $\mathbb{R}^d$ which can be represented pointwise by its power series. These functions f can be considered to arise from a multivariate expected value (3.1) with $A = I$.

An underlying motivation of this work is the common observation that QMC methods often perform well even for integrands that do not have the square-integrable mixed first derivatives as assumed in [56] (as is indeed the case for the finance problem in [49]); another motivation is the observation that QMC methods usually perform no worse than MC methods even for very difficult integrands f. The latter property, though not often mentioned, attests to an unremarked robustness of QMC methods.

3.1 The function space

In this section we define a reproducing kernel Hilbert space of functions in $(0,1)^d$ which contains functions that blow up near the boundary. These functions correspond to a large class of power series in $\mathbb{R}^d$, including some exponential functions, and are analogous to the Taylor space setting introduced by Dick [9]. The singularities are the result of using the cumulative inverse normal transformation to map the original integrand $g(\boldsymbol{u})\rho_d(\boldsymbol{u})$ in $\mathbb{R}^d$ to the unit cube $[0,1]^d$, where the integrand becomes $g(\Phi_d^{-1}(\boldsymbol{x}))$ which may be unbounded. We start by considering the one-dimensional case.

3.1.1 The univariate case

Consider the expected value

$$I_\rho(g) = \int_{\mathbb{R}} g(u)\tfrac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{u^2}{2}}\,\mathrm{d}u. \tag{3.4}$$

We wish to define a space of functions g on $\mathbb{R}$ which includes at least all polynomials,

$$g(u) = a_0 + a_1 u + \cdots + a_m u^m,$$

together with a large class of power series

$$g(u) = \sum_{k=0}^{\infty} a_k u^k \tag{3.5}$$

with infinite radius of convergence. In particular, the space should include the exponential functions

$$\mathrm{e}^{\lambda u} = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} u^k$$

for all values of λ.

Let $(\beta_1, \beta_2, \ldots)$ be a sequence of positive numbers such that $\beta_k \to 0$ and $\beta_{k+1}/\beta_k \to 0$ as $k \to \infty$. Formally, we define $\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ to be the space of all real-valued functions on $\mathbb{R}$ which are represented pointwise by their power series (3.5) and have finite norms

$$\|g\|^2_{\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{a_k^2}{\beta_k} < \infty.$$

The space $\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ is a Hilbert space with the inner product

$$\langle g, \tilde{g} \rangle_{\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{a_k \tilde{a}_k}{\beta_k}.$$

The sequence $(\beta_1, \beta_2, \ldots)$ will later be completely determined by a single parameter α which is included as a subscript in $\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$.

Note that the norm and the inner product for functions in $\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ are defined in terms of the coefficients a_k in their power-series representations (3.5).

Now we use the substitution $x = \Phi(u)$ to map the integral (3.4) over $\mathbb{R}$ into the unit interval $(0, 1)$. The resulting integral is

$$\int_0^1 f(x)\,\mathrm{d}x,$$

where the transformed integrand $f(x)$ is of the form

$$f(x) = g(\Phi^{-1}(x)) = \sum_{k=0}^{\infty} a_k [\Phi^{-1}(x)]^k, \quad x \in (0, 1). \tag{3.6}$$

Note that f is defined over the open unit interval $(0, 1)$ because it is unbounded at 0 and 1. Thus we obtain a Hilbert space $H_{\mathrm{pow},1,\alpha,\gamma}$ of functions f which is isomorphic to $\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ of functions g, and which consists of $C^\infty(0, 1)$ functions f with norm given by

$$\|f\|^2_{H_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{a_k^2}{\beta_k} < \infty,$$

and inner product given by

$$\left\langle f, \tilde{f} \right\rangle_{H_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{a_k \tilde{a}_k}{\beta_k}.$$

We stress at this point that the a_k's are the coefficients in the power-series representation of the function $g \in \mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ which is related to the function $f \in H_{\mathrm{pow},1,\alpha,\gamma}$ by (3.6).

The function

$$K_{\mathrm{pow},1,\alpha,\gamma}(x, y) = \sum_{k=0}^{\infty} \beta_k [\Phi^{-1}(x)]^k [\Phi^{-1}(y)]^k, \quad x, y \in (0, 1),$$

is the reproducing kernel in $H_{\mathrm{pow},1,\alpha,\gamma}$. Indeed we have

$$\|K_{\mathrm{pow},1,\alpha,\gamma}(x,\cdot)\|^2_{H_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{(\beta_k[\Phi^{-1}(x)]^k)^2}{\beta_k} = \sum_{k=0}^{\infty} \beta_k[\Phi^{-1}(x)]^{2k}, \ x \in (0,1),$$

which is finite by the ratio test since $\beta_{k+1}/\beta_k \to 0$ as $k \to \infty$, proving that $K_{\mathrm{pow},1,\alpha,\gamma}(x,\cdot) \in H_{\mathrm{pow},1,\alpha,\gamma}$ for all $x \in (0,1)$. Clearly $K_{\mathrm{pow},1,\alpha,\gamma}(x,y) = K_{\mathrm{pow},1,\alpha,\gamma}(y,x)$ for all $x, y \in (0,1)$. Moreover we have, for all $x \in (0,1)$ and f of the form (3.6),

$$\langle f, K_{\mathrm{pow},1,\alpha,\gamma}(x,\cdot)\rangle_{H_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{a_k\beta_k[\Phi^{-1}(x)]^k}{\beta_k} = \sum_{k=0}^{\infty} a_k[\Phi^{-1}(x)]^k = f(x),$$

which proves the reproducing property.

To ensure that the functions $f(x) = g(\Phi^{-1}(x))$ corresponding to the exponential functions $g(w) = \mathrm{e}^{\lambda w}$ are included in the space for all values of λ, we can choose

$$\beta_k = \frac{\alpha^k}{k!}, \tag{3.7}$$

where $\alpha > 0$ and $0! = 1$. Since the power-series representation of $g(u) = \mathrm{e}^{\lambda u}$ is

$$\mathrm{e}^{\lambda u} = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} u^k,$$

we can easily verify that our choice (3.7) of the β_k's leads to

$$\|f\|^2_{H_{\mathrm{pow},1,\alpha,\gamma}} = \|g\|^2_{\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}} = \sum_{k=0}^{\infty} \frac{(\frac{\lambda^k}{k!})^2}{\frac{\alpha^k}{k!}} = \sum_{k=0}^{\infty} \frac{\frac{\lambda^{2k}}{\alpha^k}}{k!} = \mathrm{e}^{\frac{\lambda^2}{\alpha}} < \infty.$$

One major benefit from our choice (3.7) of the β_k's is that the reproducing kernel can be written in a simple closed form,

$$K_{\mathrm{pow},1,\alpha,\gamma}(x,y) = \mathrm{e}^{\alpha\Phi^{-1}(x)\Phi^{-1}(y)}.$$

3.1.2 The multivariate case

Now we turn to general $d \geq 1$ and define a d-dimensional space on $(0,1)^d$ to be a tensor product of d univariate spaces $H_{\mathrm{pow},1,\alpha,\gamma}$. At the same time we introduce *weights* in the manner of [56] to allow more flexibility. Note once

again that the functions are defined over the open unit cube $(0,1)^d$ because they are unbounded near the boundaries.

Let $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ be the reproducing kernel Hilbert space with the reproducing kernel

$$K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{d}\left(\sum_{k=0}^{\infty}\beta_{k,j}[\Phi^{-1}(x_j)]^k[\Phi^{-1}(y_j)]^k\right),$$

where, for each $j = 1,\ldots,d$, we choose

$$\beta_{0,j} = 1 \quad \text{and} \quad \beta_{k,j} = \gamma_j\frac{\alpha^k}{k!} \text{ for } k \geq 1,$$

with $\alpha > 0$ and $\boldsymbol{\gamma} = (\gamma_1,\gamma_2,\ldots)$ a non-increasing sequence of positive numbers. This choice of the $\beta_{k,j}$'s ensures that the series in the definition of $K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})$ is always convergent. The space $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ consists of functions of the form

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{N}^d} a_{\boldsymbol{k}}[\Phi^{-1}(x_1)]^{k_1}\cdots[\Phi^{-1}(x_d)]^{k_d},$$

with norm given by

$$\|f\|^2_{H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}} = \sum_{\boldsymbol{k}\in\mathbb{N}^d}\frac{a_{\boldsymbol{k}}^2}{\beta_{k_1,1}\cdots\beta_{k_d,d}} < \infty,$$

and inner product

$$\left\langle f,\tilde{f}\right\rangle_{H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}} = \sum_{\boldsymbol{k}\in\mathbb{N}^d}\frac{a_{\boldsymbol{k}}\tilde{a}_{\boldsymbol{k}}}{\beta_{k_1,1}\cdots\beta_{k_d,d}}. \tag{3.8}$$

In particular, $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ includes those functions on $(0,1)^d$ which correspond to exponential functions in $\mathbb{R}^d$ of the form

$$g(\boldsymbol{u}) = \mathrm{e}^{\boldsymbol{\lambda}\cdot\boldsymbol{u}} = \prod_{j=1}^{d}\mathrm{e}^{\lambda_j u_j}$$

for all real values of the λ_j's. Moreover, it is easy to see that functions corresponding to $\tilde{g}(\boldsymbol{u}) = g(A\boldsymbol{u}+\boldsymbol{b})$ also belong to $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$, where A is a $d\times d$ matrix and $\boldsymbol{b}$ is a d-dimensional vector.

Our choice of the $\beta_{k,j}$'s leads to a simple form for the reproducing kernel

$$\begin{aligned} K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) &= \prod_{j=1}^{d}\left(1+\gamma_j\sum_{k=1}^{\infty}\frac{\alpha^k}{k!}\left[\Phi^{-1}(x_j)\right]^k\left[\Phi^{-1}(y_j)\right]^k\right) \\ &= \prod_{j=1}^{d}\left(1+\gamma_j\left[\mathrm{e}^{\alpha\Phi^{-1}(x_j)\Phi^{-1}(y_j)}-1\right]\right), \end{aligned}$$

from which it can be easily shown that for $\alpha \in (0, 1/2)$

$$\int_{[0,1]^d} K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \prod_{j=1}^{d}\left(1+\gamma_j\left(\tfrac{1}{\sqrt{1-2\alpha}}-1\right)\right).$$

To see this, note that

$$\int_0^1 \mathrm{e}^{\alpha\left[\Phi^{-1}(x)\right]^2}\,\mathrm{d}x = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{1}{2}(1-2\alpha)u^2}\,\mathrm{d}u = \frac{1}{\sqrt{1-2\alpha}}.$$

Similarly,

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

These two integrals appear in our analysis later. To ensure that they are finite, we shall assume throughout this chapter that

$$0 < \alpha < \tfrac{1}{2}.$$

We shall make use of the *shift-invariant kernel* associated with the reproducing kernel $K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y})$,

$$\begin{aligned} K^{\mathrm{sh}}_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) &= \int_{[0,1]^d} K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta} \\ &= \prod_{j=1}^{d}\left(1+\gamma_j\left[\omega(\{x_j-y_j\})-1\right]\right), \end{aligned}$$

where

$$\begin{aligned} \omega(t) &= \int_0^1 \mathrm{e}^{\alpha\Phi^{-1}(u)\Phi^{-1}(\{u+t\})}\,\mathrm{d}u \\ &= \int_0^{1-t} \mathrm{e}^{\alpha\Phi^{-1}(u)\Phi^{-1}(u+t)}\,\mathrm{d}u + \int_{1-t}^1 \mathrm{e}^{\alpha\Phi^{-1}(u)\Phi^{-1}(u+t-1)}\,\mathrm{d}u. \end{aligned} \tag{3.9}$$

We list here a few useful properties of the function ω. These properties are mostly straightforward, although some require tedious calculations.

Lemma 3.1.1 *For $0 < \alpha < \frac{1}{2}$, the function ω defined by (3.9), for $t \in [0,1]$ has the following properties:*

1. *ω is continuous over $t \in [0,1]$*
2. *$\omega(t) > 0$ for all $t \in [0,1]$*
3. *$\omega(1-t) = \omega(t)$, i.e., ω is symmetric about $t = \frac{1}{2}$*
4. *$\omega(0) = \omega(1) = \frac{1}{\sqrt{1-2\alpha}}$*
5. *$\int_0^1 \omega(t)\,\mathrm{d}t = \frac{1}{\sqrt{1-\alpha^2}}$*
6. *ω and its derivatives can be written as*

$$\begin{aligned}
\omega(t) &= 2\Upsilon(t) + 2\Upsilon(1-t),\\
\omega'(t) &= 2\Upsilon'(t) - 2\Upsilon'(1-t),\\
\omega''(t) &= 2\Upsilon''(t) + 2\Upsilon''(1-t),
\end{aligned}$$

where

$$\begin{aligned}
\Upsilon(t) &= \int_{-\infty}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} \mathrm{e}^{\alpha u \Phi^{-1}(\Phi(u)+t)} \tfrac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{u^2}{2}}\,\mathrm{d}u,\\
\Upsilon'(t) &= \int_{-\infty}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} \alpha u \mathrm{e}^{\frac{1}{2}[\Phi^{-1}(\Phi(u)+t)]^2 + \alpha u \Phi^{-1}(\Phi(u)+t) - \frac{u^2}{2}}\,\mathrm{d}u - \tfrac{1}{2}\mathrm{e}^{-\alpha\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2},\\
\frac{\Upsilon''(t)}{\sqrt{2\pi}\alpha} &= \int_{-\infty}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} u[\Phi^{-1}(\Phi(u)+t)+\alpha u]\mathrm{e}^{[\Phi^{-1}(\Phi(u)+t)]^2 + \alpha u \Phi^{-1}(\Phi(u)+t) - \frac{u^2}{2}}\,\mathrm{d}u\\
&\quad - \Phi^{-1}\left(\tfrac{1-t}{2}\right) \mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2}.
\end{aligned}$$

7. *$\omega''(t) \geq 0$ for all $t \in [0,1]$.*

Proof. Parts 1–5 are elementary. To prove part 6, we write $\omega(t)$ as a sum of four integrals:

$$\begin{aligned}
\omega(t) = &\int_0^{\frac{1-t}{2}} \mathrm{e}^{\alpha\Phi^{-1}(x)\Phi^{-1}(x+t)}\,\mathrm{d}x + \int_{\frac{1-t}{2}}^{1-t} \mathrm{e}^{\alpha\Phi^{-1}(x)\Phi^{-1}(x+t)}\,\mathrm{d}x\\
&+ \int_{1-t}^{1-\frac{t}{2}} \mathrm{e}^{\alpha\Phi^{-1}(x)\Phi^{-1}(x+t-1)}\,\mathrm{d}x + \int_{1-\frac{t}{2}}^{1} \mathrm{e}^{\alpha\Phi^{-1}(x)\Phi^{-1}(x+t-1)}\,\mathrm{d}x.
\end{aligned}$$

To remove the singularities at the boundaries, we use a different substitution for each integral:

first integral	$u = \Phi^{-1}(x)$,	second integral	$u = -\Phi^{-1}(x+t)$,
third integral	$u = \Phi^{-1}(x+t-1)$,	fourth integral	$u = -\Phi^{-1}(x)$.

These substitutions, together with the property $-\Phi^{-1}(x) = \Phi^{-1}(1-x)$, lead to the new expression for $\omega(t)$ in terms of the integral $\Upsilon(t)$. The expressions for $\Upsilon'(t)$ and $\Upsilon''(t)$ can be obtained using Leibniz's formula.

To prove part 7, it suffices to show that

$$\frac{\Upsilon''(t)}{\sqrt{2\pi}\alpha} = \int_{-\infty}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} q(u) u \mathrm{e}^{-\frac{u^2}{2}} \,\mathrm{d}u - \Phi^{-1}\left(\tfrac{1-t}{2}\right) \mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2}$$

is non-negative, where

$$q(u) = \left(\Phi^{-1}(\Phi(u)+t) + \alpha u\right) \mathrm{e}^{\Phi^{-1}(\Phi(u)+t)[\Phi^{-1}(\Phi(u)+t)+\alpha u]}$$

for $-\infty < u \le \Phi^{-1}(\frac{1-t}{2}) \le 0$. First we observe that $\Phi^{-1}(\Phi(u)+t) + \alpha u$ is monotonically increasing in u, with a limit of $-\infty$ as $u \to -\infty$ and a value of $(1-\alpha)\Phi^{-1}(\frac{1+t}{2}) \ge 0$ at the upper limit $u = \Phi^{-1}(\frac{1-t}{2})$. Thus there exists some $-\infty < \overline{u} \le \Phi^{-1}(\frac{1-t}{2}) \le 0$ such that $\Phi^{-1}(\Phi(\overline{u})+t) + \alpha\overline{u} = 0$. Clearly $u\mathrm{e}^{-u^2/2} \le 0$ for all $u \le 0$, $q(u) \le 0$ for $u \le \overline{u}$, and $q(u) \ge 0$ for $u \ge \overline{u}$. By splitting the integral into two and dropping the one with the positive integrand, we can write

$$\begin{aligned}
\frac{\Upsilon''(t)}{\sqrt{2\pi}\alpha} &= \int_{-\infty}^{\overline{u}} q(u) u \mathrm{e}^{-\frac{u^2}{2}} \,\mathrm{d}u + \int_{\overline{u}}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} q(u) u \mathrm{e}^{-\frac{u^2}{2}} \,\mathrm{d}u \\
&\quad - \Phi^{-1}\left(\tfrac{1-t}{2}\right) \mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2} \\
&\ge \int_{\overline{u}}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} q(u) u \mathrm{e}^{-\frac{u^2}{2}} \,\mathrm{d}u - \Phi^{-1}\left(\tfrac{1-t}{2}\right) \mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2}.
\end{aligned}$$

For $\overline{u} \leq u \leq \Phi^{-1}(\frac{1-t}{2})$, $q(u) \geq 0$ attains its maximum at $u = \Phi^{-1}(\frac{1-t}{2})$. Thus

$$\begin{aligned}
\frac{\Upsilon''(t)}{\sqrt{2\pi}\alpha} &\geq q\left(\Phi^{-1}\left(\tfrac{1-t}{2}\right)\right) \int_{\overline{u}}^{\Phi^{-1}\left(\frac{1-t}{2}\right)} u\mathrm{e}^{-\frac{u^2}{2}}\,\mathrm{d}u - \Phi^{-1}\left(\tfrac{1-t}{2}\right)\mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1-t}{2}\right)\right]^2} \\
&= (1-\alpha)\Phi^{-1}\left(\tfrac{1+t}{2}\right)\mathrm{e}^{(1-\alpha)\left[\Phi^{-1}\left(\frac{1+t}{2}\right)\right]^2}\left(\mathrm{e}^{-\frac{\overline{u}^2}{2}} - \mathrm{e}^{-\frac{1}{2}\left[\Phi^{-1}\left(\frac{1+t}{2}\right)\right]^2}\right) \\
&\quad + \Phi^{-1}\left(\tfrac{1+t}{2}\right)\mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1+t}{2}\right)\right]^2} \\
&= (1-\alpha)\Phi^{-1}\left(\tfrac{1+t}{2}\right)\mathrm{e}^{(1-\alpha)\left[\Phi^{-1}\left(\frac{1+t}{2}\right)\right]^2 - \frac{\overline{u}^2}{2}} + \alpha\Phi^{-1}\left(\tfrac{1+t}{2}\right)\mathrm{e}^{(\frac{1}{2}-\alpha)\left[\Phi^{-1}\left(\frac{1+t}{2}\right)\right]^2} \\
&\geq 0.
\end{aligned}$$

This concludes the proof. □

See Figure 3.2 for the graphs of $\omega(t)$, $\omega'(t)$ and $\omega''(t)$ when $\alpha = 0.375$.

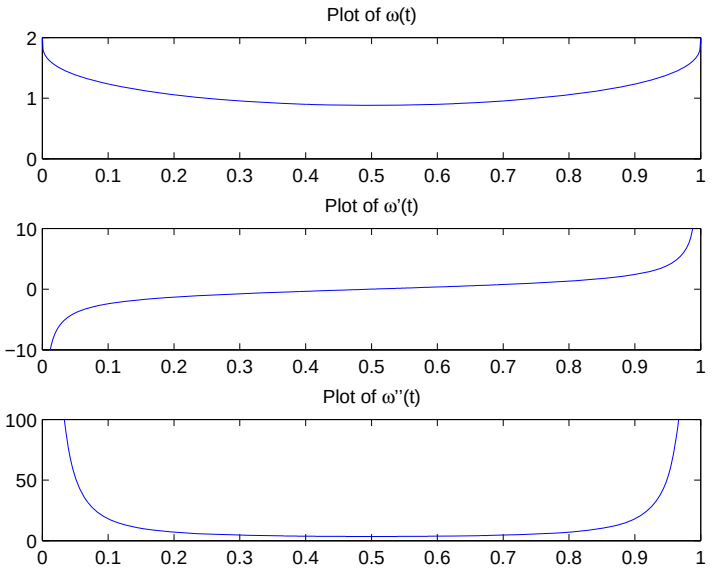

Figure 3.2: Graph of $\omega(t)$, $\omega'(t)$ and $\omega''(t)$ for $\alpha = 0.375$

3.2 Worst-case error analysis

Using the theory developed in Section 2.3, we can write down the worst-case error $e_{n,d}(P_{n,d}; K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}})$ for a given point set in this new space, as well as the

QMC mean $M_{n,d}$. We begin by noting that

$$\begin{aligned}\|f\|_{L_2([0,1]^d)} &= \left(\int_{[0,1]^d} f^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\right)^{1/2} \\ &\le \left(\int_{[0,1]^d} K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\right)^{1/2} \|f\|_{H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}}.\end{aligned}$$

Note that since $\alpha \in (0,1/2)$ we have

$$\int_{[0,1]^d} K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} < \infty$$

to ensure that $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ is embedded in $L_2([0,1]^d)$. This assumption also ensures that the initial error $e^2_{0,d}(K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}})$ in $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ is finite and $M_{n,d} < \infty$.

For our function space $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$, I_d is well defined, with the representer

$$\xi_{n,d}(\boldsymbol{x}) = \prod_{j=1}^{d} \left(1 + \gamma_j \left(\mathrm{e}^{\frac{1}{2}\alpha^2[\Phi^{-1}(x_j)]^2} - 1\right)\right).$$

To simplify our notations, we define for $s \in (0,1)$,

$$\eta_s = \frac{1}{\sqrt{1-s}} - 1.$$

Thus we have $\omega(0) = \omega(1) = 1 + \eta_{2\alpha}$ and $\int_0^1 \omega(t)\,\mathrm{d}t = 1 + \eta_{\alpha^2}$. The initial error in $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ is

$$e_{0,d}(K_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}) = \prod_{j=1}^{d} (1 + \gamma_j \eta_{\alpha^2})^{1/2},$$

and the squared QMC mean is

$$M^2_{\mathrm{pow},n,d,\boldsymbol{\gamma}} = \frac{1}{n}\left(\prod_{j=1}^{d}(1+\gamma_j\eta_{2\alpha}) - \prod_{j=1}^{d}(1+\gamma_j\eta_{\alpha^2})\right). \tag{3.10}$$

In this chapter, we shall denote the worst-case error for a lattice rule with generating vector $\boldsymbol{z}$ and shift $\boldsymbol{\Delta}$ by $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z},\boldsymbol{\Delta})$. If the shift $\boldsymbol{\Delta}$ is taken to be randomly chosen, then we shall denote the expected worst-case error for the randomly-shifted lattice rule by $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$.

The squared worst-case error for randomly-shifted rank-1 lattice rules in $H_{\mathrm{pow},d,\alpha,\boldsymbol{\gamma}}$ is given by

$$\begin{aligned} e^2_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) &= \int_{[0,1]^d} e^2_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z},\boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta} \\ &= -\prod_{j=1}^{d}(1+\gamma_j\eta_{\alpha^2}) + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1+\gamma_j\left[\omega\left(\left\{\frac{kz_j}{n}\right\}\right)-1\right]\right). \end{aligned} \tag{3.11}$$

3.2.1 The existence of good generating vectors

We are now in a position to assess the potential of randomly-shifted rank-1 lattice rules. Theorem 3.2.2 below proves the existence of a generating vector for which the worst-case error is smaller than the QMC mean. The proof of this theorem relies on the following lemma. Again, we will only consider the case where $n = p^m$ is the power of a prime p.

Lemma 3.2.1 *Let $\omega(t)$ be defined as in (3.9) and $n = p^m$ be the power of a prime p. Then*

$$\frac{1}{\phi(p^m)}\sum_{z\in\mathcal{Z}_{p,m}}\omega\left(\tfrac{z}{p^m}\right) < \int_0^1 \omega(t)\,\mathrm{d}t = 1+\eta_{\alpha^2},$$

with $\mathcal{Z}_{p,m}$ defined by (2.34) for $d = 1$.

This was shown for the case where n is prime in [65]. Here, we extend the lemma for powers of a prime.

Proof. We begin by noting that the result is trivial if $p = 2$. In this case

$$\frac{1}{\phi(p^m)}\sum_{z\in\mathcal{Z}_{p,m}}\omega\left(\tfrac{z}{p^m}\right)$$

is a midpoint-rule approximation of

$$\int_0^1 \omega(t)\,\mathrm{d}t.$$

The convexity of ω means that the midpoint rule will underestimate the integral and so the inequality holds. For the case where p is an odd prime, we can use

the symmetry of $\omega(t)$ about $t = 1/2$ to write the left-hand side of the lemma as

$$\begin{aligned}
&\frac{1}{\phi(p^m)} \sum_{z \in \mathcal{Z}_{p,m}} \omega\left(\tfrac{z}{p^m}\right) \\
&= \frac{1}{\phi(p^m)} \sum_{k=0}^{p^{m-1}-1} \sum_{i=1}^{p-1} \omega\left(\tfrac{kp+i}{p^m}\right) \\
&= \frac{2}{\phi(p^m)} \sum_{k=0}^{(p^{m-1}-3)/2} \sum_{i=1}^{p-1} \omega\left(\tfrac{kp+i}{p^m}\right) + \frac{1}{\phi(p^m)} \sum_{i=1}^{p-1} \omega\left(\tfrac{1}{2} + \tfrac{2i-p}{2p^m}\right). \qquad (3.12)
\end{aligned}$$

We will now treat each of the two parts of the last line separately. Beginning with the second part, we define a mapping $\varphi_{p,m}(t)$ by

$$\varphi_{p,m}(t) = \tfrac{p}{p-1}\left(t - \tfrac{1}{2}\right) + \tfrac{1}{2}.$$

Clearly $\varphi_{p,m}(\frac{1}{2}) = \frac{1}{2}$, $\varphi_{p,m}(t) < t$ if $t < \frac{1}{2}$ and $\phi_{p,m}(t) > t$ if $t > \frac{1}{2}$. Therefore, it follows by the convexity of ω that

$$\begin{aligned}
\frac{1}{\phi(p^m)} \sum_{i=1}^{p-1} \omega\left(\tfrac{1}{2} + \tfrac{2i-p}{2p^m}\right) &< \frac{1}{p^{m-1}} \frac{1}{p-1} \sum_{i=1}^{p-1} \omega\left(\varphi_{p,m}\left(\tfrac{1}{2} + \tfrac{2i-p}{2p^m}\right)\right) \\
&= \frac{1}{p^{m-1}} \frac{1}{p-1} \sum_{i=1}^{p-1} \omega\left(\tfrac{1}{2} + \tfrac{2i-p}{2p^{m-1}(p-1)}\right) \\
&< \int_{\frac{1}{2}-\frac{1}{2p^m}}^{\frac{1}{2}+\frac{1}{2p^m}} \omega(t)\,\mathrm{d}t.
\end{aligned}$$

Looking now at the first part of (3.12), we see that ω is always monotonic decreasing. We will exploit this by writing each term in the sum for $k = 0, \ldots, \frac{p^m-3}{2}$ as

$$\frac{1}{\phi(p^m)} \sum_{i=1}^{(p-1)/2} \left(\omega\left(\tfrac{kp+i}{p^m}\right) + \omega\left(\tfrac{kp+p-i}{p^m}\right)\right).$$

As before, consider the mapping

$$\varphi_{p,m,k}(t) = \tfrac{p}{p-1}\left(t - \tfrac{2k+1}{2p^{m-1}}\right) + \tfrac{2k+1}{2p^{m-1}}.$$

For a given $k \in \{0, \ldots, \frac{p^m-3}{2}\}$ and for $i = 1, \ldots, \frac{p-1}{2}$ we can see by the monotonicity of ω that

$$\omega\left(\tfrac{kp+i}{p^m}\right) < \omega\left(\varphi_{p,m,k}\left(\tfrac{kp+i}{p^m}\right)\right)$$

and

$$\omega\left(\tfrac{kp+p-i}{p^m}\right) > \omega\left(\varphi_{p,m,k}\left(\tfrac{kp+p-i}{p^m}\right)\right).$$

However, since ω is also concave up, it follows that

$$\omega\left(\varphi_{p,m,k}\left(\tfrac{kp+i}{p^m}\right)\right) - \omega\left(\tfrac{kp+i}{p^m}\right) > \omega\left(\tfrac{kp+p-i}{p^m}\right) - \omega\left(\varphi_{p,m,k}\left(\tfrac{kp+p-i}{p^m}\right)\right).$$

Therefore, we can write

$$\begin{aligned}
&\frac{1}{\phi(p^m)} \sum_{i=1}^{(p-1)/2} \left(\omega\left(\tfrac{kp+i}{p^m}\right) + \omega\left(\tfrac{kp+p-i}{p^m}\right)\right) \\
&< \frac{1}{p^{m-1}} \frac{1}{p-1} \sum_{i=1}^{(p-1)/2} \left(\omega\left(\varphi_{p,m,k}\left(\tfrac{kp+i}{p^m}\right)\right) + \omega\left(\varphi_{p,m,k}\left(\tfrac{kp+p-i}{p^m}\right)\right)\right) \\
&= \frac{1}{p^{m-1}} \frac{1}{p-1} \sum_{i=1}^{p-1} \omega\left(\tfrac{2k+1}{2p^{m-1}} + \tfrac{2i-p}{2p^{m-1}(p-1)}\right) \\
&< \int_{\frac{k}{p^{m-1}}}^{\frac{k+1}{p^{m-1}}} \omega(t)\,\mathrm{d}t.
\end{aligned}$$

Taking this over all values of k gives the result. □

We now prove, by means of an averaging argument, that for $n = p^m$ there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$ such that the worst-case error of the randomly-shifted lattice rule is smaller than the QMC mean.

Theorem 3.2.2 *For $n = p^m$ the power of a prime p and $\alpha \in (0, 1/2)$, there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$ such that*

$$e_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) < M_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}$$

Proof. Averaging $e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ (see (3.11)) over all possible $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$ and separating out the $k = p^m$ term, we obtain

$$\begin{aligned}
&\frac{1}{\phi(p^m)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_{p,m}^d} e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \\
&= -\prod_{j=1}^{d} (1 + \gamma_j \eta_{\alpha^2}) + \frac{1}{p^m} \prod_{j=1}^{d} (1 + \gamma_j \eta_{2\alpha}) \\
&\quad + \frac{1}{p^m} \sum_{k=1}^{p^m-1} \prod_{j=1}^{d} \left(1 + \gamma_j \left[\frac{1}{\phi(p^m)} \sum_{z_j \in \mathcal{Z}_{p,m}} \omega\left(\left\{\frac{kz_j}{p^m}\right\}\right) - 1\right]\right).
\end{aligned}$$

We note that for a given $1 \leq k \leq p^m - 1$, the set

$$\left\{ \left\{ \frac{kz_j}{p^m} \right\} : z_j \in \mathcal{Z}_{p,m} \right\}$$

is p^ℓ copies of the set

$$\left\{ \left\{ \frac{z_j}{p^{m-\ell}} \right\} : z_j \in \mathcal{Z}_{p,m-\ell} \right\}$$

where ℓ is the largest integer such that $p^\ell | k$. Therefore, we may use this and Lemma 3.2.1 to write

$$\frac{1}{\phi(p^m)} \sum_{z_j \in \mathcal{Z}_{p,m}} \omega\left(\left\{ \frac{kz_j}{p^m} \right\} \right) - 1 = \frac{1}{\phi(p^{m-\ell})} \sum_{z \in \mathcal{Z}_{p,m-\ell}} \omega\left(\left\{ \frac{z_j}{p^{m-\ell}} \right\} \right) - 1 < \eta_{\alpha^2}, \tag{3.13}$$

which leads to

$$\begin{aligned}
&\frac{1}{\phi(p^m)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_{p,m}^d} e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \\
&< -\prod_{j=1}^{d} (1 + \gamma_j \eta_{\alpha^2}) + \frac{1}{p^m} \prod_{j=1}^{d} (1 + \gamma_j \eta_{2\alpha}) + \frac{p^m - 1}{p^m} \prod_{j=1}^{d} (1 + \gamma_j \eta_{\alpha^2}) \\
&= M^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}.
\end{aligned}$$

with $M^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}$ given by (3.10). Thus there exists a $\boldsymbol{z}$ for which the squared worst-case error is smaller than the average, and in turn smaller than the squared QMC mean. □

We can obtain a lower bound on $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ following the technique used in Section 2.4.2.

Theorem 3.2.3 *For $n = p^m$ the power of a prime p, $\alpha \in (0, 1/2)$ and any generating vector $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$, we have*

$$e^2_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \geq -\prod_{j=1}^{d} (1 + \kappa \gamma_j \eta_{\alpha^2}) + \frac{1}{n} \prod_{j=1}^{d} (1 + \kappa \gamma_j \eta_{2\alpha}),$$

where

$$\kappa = \min\left(1, \frac{1}{\gamma_1 |\, \omega(\frac{1}{2}) - 1 \,|}\right).$$

Proof. Let $\bar{\boldsymbol{\gamma}} = (\bar{\gamma}_1, \bar{\gamma}_2, \ldots)$ be a non-increasing sequence given by $\bar{\gamma}_j = \kappa\gamma_j$, where κ is as defined in the theorem. Then it is not hard to verify that for each $j = 1, \ldots, d$ we have

$$\bar{\gamma}_j \leq \gamma_j \quad \text{and} \quad 1 + \bar{\gamma}_j \left[\omega(t) - 1 \right] \geq 0 \quad \text{for all } t \in [0, 1],$$

where the second condition follows from the property that $\omega(t)$ has its minimum at $t = 1/2$.

Since the new weights $\bar{\boldsymbol{\gamma}}$ are no larger than $\boldsymbol{\gamma}$, the unit ball of the space weighted by $\bar{\boldsymbol{\gamma}}$ is contained in the unit ball of the space weighted by $\bar{\boldsymbol{\gamma}}$ and thus it follows from the definition of worst-case error and the expression (3.11), with γ_j replaced by $\bar{\gamma}_j$, that

$$\begin{aligned} e^2_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) &\geq e^2_{\mathrm{pow},n,d,\alpha,\bar{\boldsymbol{\gamma}}}(\boldsymbol{z}) \\ &= -\prod_{j=1}^{d} (1 + \bar{\gamma}_j \eta_{\alpha^2}) + \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(1 + \bar{\gamma}_j \left[\omega\left(\left\{ \frac{k z_j}{n} \right\} \right) - 1 \right] \right). \end{aligned}$$

This last expression includes a sum over non-negative terms and thus a lower bound can be obtained by keeping only the $k = 0$ term in the sum. This leads to the lower bound stated in the theorem. □

From the upper and lower bounds established in Theorems 3.2.2 and 3.2.3, we may conclude that the condition $\sum_{j=1}^{\infty} \gamma_j < \infty$ is both necessary and sufficient for $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ to be bounded independently of d.

Theorem 3.2.4 *If $\sum_{j=1}^{\infty} \gamma_j < \infty$, then for $n = p^m$ the power of a prime p there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}^d_{p,m}$ such that*

$$e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) < \frac{c}{\sqrt{n}} \qquad \textit{for all } d = 1, 2, \ldots,$$

where c is independent of n and d. On the other hand if $\sum_{j=1}^{\infty} \gamma_j = \infty$, then $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ grows to infinity as $d \to \infty$ for all $n = p^m$ and all $\boldsymbol{z} \in \mathcal{Z}^d_{p,m}$.

The proof is similar to that given in Section 2.4.2, and relies on Theorem 3.2.3.

Proof. It follows from Theorem 3.2.2 that there exists a $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$, where for $n = p^m$

$$\begin{aligned} e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) < M_{\mathrm{pow},n,d,\boldsymbol{\gamma}} &< \frac{1}{\sqrt{n}} \prod_{j=1}^{d} \left(1 + \gamma_j \eta_{2\alpha}\right)^{1/2} \\ &= \frac{1}{\sqrt{n}} \exp\left(\frac{1}{2} \sum_{j=1}^{d} \log\left(1 + \gamma_j \eta_{2\alpha}\right)\right) \\ &\leq \frac{1}{\sqrt{n}} \exp\left(\frac{\eta_{2\alpha}}{2} \sum_{j=1}^{\infty} \gamma_j\right). \end{aligned}$$

Thus we have $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) < cn^{-1/2}$, where c is bounded independently of d if $\sum_{j=1}^{\infty} \gamma_j < \infty$.

Now we prove the necessity of $\sum_{j=1}^{\infty} \gamma_j < \infty$. It follows from Theorem 3.2.3 that

$$e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \geq \prod_{j=1}^{d} \left(1 + \kappa\gamma_j \eta_{\alpha^2}\right)^{1/2} \left[\frac{1}{n} \prod_{j=1}^{d} \left(\frac{1 + \kappa\gamma_j \eta_{2\alpha}}{1 + \kappa\gamma_j \eta_{\alpha^2}}\right) - 1\right]^{1/2}. \tag{3.14}$$

We begin by finding a lower bound on the term

$$\prod_{j=1}^{d} \left(1 + \kappa\gamma_j \eta_{\alpha^2}\right) = \exp\left(\sum_{j=1}^{d} \log(1 + \kappa\gamma_j \eta_{\alpha^2})\right).$$

Consider the function

$$\Psi(x) = \log(1 + x) - b_\alpha x, \quad \text{where } b_\alpha = \frac{\log(1 + \kappa\gamma_1 \eta_{\alpha^2})}{\kappa\gamma_1 \eta_{\alpha^2}}.$$

Clearly

$$\Psi(0) = 0, \quad \Psi(\kappa\gamma_1 \eta_{\alpha^2}) = 0 \quad \text{and} \quad \Psi''(x) = -\frac{1}{(1 + x)^2} < 0.$$

Therefore, for $x \in [0, \kappa\gamma_1 \eta_{\alpha^2}]$, $\log(1 + x) \geq b_\alpha x$. Since $\gamma_1 \geq \gamma_j$ for all $j = 1, \ldots, d$, we may write

$$\prod_{j=1}^{d} \left(1 + \kappa\gamma_j \eta_{\alpha^2}\right) \geq \exp\left(\frac{\log(1 + \kappa\gamma_1 \eta_{\alpha^2})}{\gamma_1} \sum_{j=1}^{d} \gamma_j\right).$$

Similarly, we can show that a lower bound of the second product in (3.14) is

$$\begin{aligned} \prod_{j=1}^{d} \left(\frac{1 + \kappa\gamma_j \eta_{2\alpha}}{1 + \kappa\gamma_j \eta_{\alpha^2}}\right) &\geq \prod_{j=1}^{d} \left(1 + \frac{\kappa(\eta_{2\alpha} - \eta_{\alpha^2})}{1 + \kappa\gamma_1 \eta_{\alpha^2}} \gamma_j\right) \\ &\geq \exp\left(\frac{1}{\gamma_1} \log\left(1 + \frac{\kappa\gamma_1(\eta_{2\alpha} - \eta_{\alpha^2})}{1 + \kappa\gamma_1 \eta_{\alpha^2}}\right) \sum_{j=1}^{d} \gamma_j\right). \end{aligned}$$

Hence if $\sum_{j=1}^{\infty} \gamma_j = \infty$, $e_{\text{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ must go to infinity as $d \to \infty$. This completes the proof. □

3.2.2 Component-by-component construction

Here we present a component-by-component (CBC) algorithm, similar to the one presented in Section 2.6.2 to construct the generating vector $\boldsymbol{z}$ based on minimising the worst-case error in each step. Theorem 3.2.5 below states that the lattice rule constructed this way has worst-case error smaller than the QMC mean.

Algorithm 2 CBC algorithm for the space of analytic functions

Require: Let $n = p^m$ be the power of a prime p, $\alpha \in (0, 1/2)$, $d_{\max}$ some integer

1: Set $z_1^* = 1$
2: **for** $d = 1$ to $d_{\max} - 1$ **do**
3: Find $z_{d+1}^* \in \mathcal{Z}_{p,m}$ which minimises $e_{\text{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))$
4: Set $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$
5: **end for**

Theorem 3.2.5 *For $n = p^m$ the power of a prime p and $\alpha \in (0, 1/2)$, the generating vector $\boldsymbol{z}_d^* = (z_1^*, \ldots, z_d^*) \in \mathcal{Z}_{p,m}^d$ constructed by Algorithm 2 satisfies*

$$e_{\text{pow},n,d,\alpha,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*) < M_{\text{pow},n,d,\boldsymbol{\gamma}}$$

for all $d = 1, 2, \ldots, d_{\max}$.

Proof. We prove this theorem by induction. For $d = 1$ we take $z_1^* = 1$, and by (3.10), (3.11) and Lemma 3.2.1

$$\begin{aligned}
&e^2_{\text{pow},p^m,1,\alpha,\gamma_1}(z_1^*) \\
&= -(1 + \gamma_1 \eta_{\alpha^2}) + \frac{1}{p^m}(1 + \gamma_1 \eta_{2\alpha}) + \frac{1}{p^m} \sum_{i=1}^{n-1} \left(1 + \gamma_1 \left[\omega\left(\frac{i}{p^m}\right) - 1\right]\right) \\
&< -(1 + \gamma_1 \eta_{\alpha^2}) + \frac{1}{p^m}(1 + \gamma_1 \eta_{2\alpha}) + \frac{p^m - 1}{p^m}(1 + \gamma_1 \eta_{\alpha^2}) = M^2_{\text{pow},p^m,1,\alpha,\gamma_1}.
\end{aligned}$$

Now assume that $e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(z_1^*,\ldots,z_d^*) < M^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}$ holds for some d. As in (2.45), we define the quantity

$$\theta_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) = e^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1})) - e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*), \quad (3.15)$$

and show that

$$\frac{1}{\phi(p^m)} \sum_{z_{d+1}\in\mathcal{Z}_{p,m}} \theta_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \le \overline{\theta}_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$$

where

$$\overline{\theta}_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) = \gamma_{d+1}\eta_{\alpha^2} e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) + \frac{\gamma_{d+1}(\eta_{2\alpha}-\eta_{\alpha^2})}{p^m}\prod_{j=1}^{d}(1+\gamma_j\eta_{2\alpha}).$$

From the definition of $\theta_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$ and (3.11) we see that

$$\begin{aligned}
&\theta_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \\
&= -\gamma_{d+1}\eta_{\alpha^2}\prod_{j=1}^{d}(1+\gamma_j\eta_{\alpha^2}) + \frac{\gamma_{d+1}\eta_{2\alpha}}{p^m}\prod_{j=1}^{d}(1+\gamma_j\eta_{2\alpha}) \\
&\quad + \frac{\gamma_{d+1}}{p^m}\sum_{k=1}^{p^m-1}\left[\left(\omega\left(\left\{\frac{kz_{d+1}}{p^m}\right\}\right)-1\right)\prod_{j=1}^{d}\left(1+\gamma_j\left[\omega\left(\left\{\frac{kz_j^*}{p^m}\right\}\right)-1\right]\right)\right].
\end{aligned}$$

As before, we recall (3.13) which showed

$$\frac{1}{\phi(p^m)}\sum_{z_j\in\mathcal{Z}_{p,m}}\omega\left(\left\{\frac{kz_j}{p^m}\right\}\right) - 1 < \eta_{\alpha^2},$$

which gives us

$$\begin{aligned}
&\frac{1}{\phi(p^m)} \sum_{z_{d+1}\in\mathcal{Z}_{p,m}} \theta_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \\
&= -\gamma_{d+1}\eta_{\alpha^2}\prod_{j=1}^{d}(1+\gamma_j\eta_{\alpha^2}) + \frac{\gamma_{d+1}\eta_{2\alpha}}{p^m}\prod_{j=1}^{d}(1+\gamma_j\eta_{2\alpha}) \\
&\quad + \frac{\gamma_{d+1}\eta_{\alpha^2}}{p^m}\sum_{k=1}^{p^m-1}\prod_{j=1}^{d}\left(1+\gamma_j\left[\omega\left(\left\{\frac{kz_j^*}{p^m}\right\}\right)-1\right]\right). \\
&= \gamma_{d+1}\eta_{\alpha^2} e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) + \frac{\gamma_{d+1}(\eta_{2\alpha}-\eta_{\alpha^2})}{p^m}\prod_{j=1}^{d}(1+\gamma_j\eta_{2\alpha}).
\end{aligned}$$

Putting this together with the inductive assumption, we obtain

$$\begin{aligned}
&\frac{1}{\phi(p^m)} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} e^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*, z_{d+1}) \\
&\le (1 + \gamma_{d+1}\eta_{\alpha^2})\, e^2_{\mathrm{pow},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) + \frac{\gamma_{d+1}(\eta_{2\alpha} - \eta_{\alpha^2})}{p^m} \prod_{j=1}^{d} (1 + \gamma_j \eta_{2\alpha}) \\
&\le \frac{1}{p^m} (1 + \gamma_{d+1}\eta_{\alpha^2}) \left(\prod_{j=1}^{d} (1 + \gamma_j \eta_{2\alpha}) + \prod_{j=1}^{d} (1 + \gamma_j \eta_{\alpha^2}) \right) \\
&\qquad + \frac{\gamma_{d+1}(\eta_{2\alpha} - \eta_{\alpha^2})}{p^m} \prod_{j=1}^{d} (1 + \gamma_j \eta_{2\alpha}) \\
&= \frac{1}{p^m} \left(\prod_{j=1}^{d+1} (1 + \gamma_j \eta_{2\alpha}) + \prod_{j=1}^{d+1} (1 + \gamma_j \eta_{\alpha^2}) \right) = M^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}.
\end{aligned}$$

Now since $z_{d+1}^* \in \mathcal{Z}_{p,m}$ is chosen to minimise $e^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*, z_{d+1})$, it must satisfy

$$\begin{aligned}
&e^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*, z_{d+1}^*) \\
&\le \frac{1}{\phi(p^m)} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} e^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*, z_{d+1}) < M^2_{\mathrm{pow},p^m,d+1,\alpha,\boldsymbol{\gamma}}.
\end{aligned}$$

This completes the proof. □

The implementation of the CBC algorithm requires the evaluation of the function

$$\omega(t) = \int_0^{1-t} e^{\alpha\Phi^{-1}(u)\Phi^{-1}(u+t)}\,\mathrm{d}u + \int_{1-t}^{1} \mathrm{e}^{\alpha\Phi^{-1}(u)\Phi^{-1}(u+t-1)}\,\mathrm{d}u,$$

at $t = \frac{i}{p^m}$ for each $i = 0, \ldots, p^m - 1$. We use the double exponential substitution first proposed in [59], that is, we use

$$u = \tfrac{1}{2}(1-t)\left[1 + \tanh\left(\tfrac{\pi}{2}\sinh w\right)\right].$$

This leads to an integral which can be evaluated using Simpson's rule with low truncation error.

The cost of constructing the n-point lattice rule for d dimensions is $O(n^2d^2)$ operations which can be reduced to $O(n^2d)$ operations by storing the product

terms during the search. This requires $O(n)$ storage. Using the fast CBC implementation of [45, 47, 46], the cost can be reduced to $O(n \log(n)\, d)$ operations.

3.3 Numerical experiments

In this section we compare the robustness and the performance of the lattice rules obtained from our new function spaces with those obtained from the unanchored weighted Sobolev spaces presented in Section 2.4.3. Recall that the worst-case error for randomly-shifted rank-1 lattice rules in the unanchored weighted Sobolev spaces is identical to the worst-case error of the weighted Korobov space with $\alpha = 2$. From (2.30) we get that this worst-case error is

$$e^2_{\mathrm{sob},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}) = -1 + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(1 + \gamma_j B_2\left(\left\{\frac{kz_j}{n}\right\}\right)\right) \tag{3.16}$$

where $B_2(x) = x^2 - x + 1/6$ is the Bernoulli polynomial of degree 2.

For these spaces, we consider five different sequences of $\boldsymbol{\gamma}$, including both decaying weights and equal weights

$$\gamma_j = \frac{1}{j^2}, \quad \gamma_j = 0.9^j, \quad \gamma_j = 0.05, \quad \gamma_j = 0.5, \quad \gamma_j = 0.9. \tag{3.17}$$

Note also that the choice of equal weights in our current tensor-product setting has an alternative interpretation – it is equivalent to having *order-dependent weights* under the more generalised setting of [55], where a weight Γ_ℓ describes the relative importance of the interactions between variables taken ℓ at a time. More precisely, having $\gamma_j = r$ in a tensor-product setting is equivalent to having $\Gamma_\ell = r^\ell$ in the order-dependent setting. By choosing $r < 1$, we are saying that the higher-order interactions are less and less important compared to the lower-order ones. Results from some experiments have indicated that lattice rules constructed according to the classical criterion P_α (see for example [51], [54]) perform poorly in some practical applications. This is not at all surprising as P_α is equivalent to taking $r = 2\pi^2$ in the tensor-product

n	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
1009	2.32e-02	2.73e-01	1.07e-02	2.07e-01	7.48e-01
2003	1.53e-02	1.91e-01	7.08e-03	1.44e-01	5.27e-01
4001	1.01e-02	1.32e-01	4.62e-03	9.96e-02	3.69e-01
8009	6.64e-03	9.18e-02	3.03e-03	6.90e-02	2.58e-01
16001	4.38e-03	6.37e-02	1.99e-03	4.76e-02	1.81e-01
32003	2.88e-03	4.41e-02	1.30e-03	3.29e-02	1.26e-01
64007	1.89e-03	3.05e-02	8.54e-04	2.27e-02	8.84e-02

Table 3.1: Worst-case errors in the new spaces

n	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
1009					
2003	0.598	0.517	0.601	0.521	0.505
4001	0.604	0.526	0.615	0.530	0.513
8009	0.602	0.529	0.609	0.530	0.515
16001	0.602	0.528	0.610	0.535	0.514
32003	0.603	0.531	0.612	0.532	0.518
64007	0.605	0.529	0.606	0.535	0.515

Table 3.2: The observed order of convergence $O(n^{-a})$ in the new spaces

setting. Thus much more emphasis is put on the higher-order interactions, which is often a very unrealistic assumption in practice.

For each sequence of weights $\boldsymbol{\gamma}$ given above and for each $n = 1009$, 2003, 4001, 8009, 16001, 32003, and 64007 (all of which are prime numbers), we construct a generating vector up to 100 dimensions using the fast CBC implementation of Algorithm 2. The worst-case errors (as defined in (3.11)) for these generating vectors and the observed order of convergence $O(n^{-a})$ are given in Tables 3.1 and 3.3 respectively. Note that the observed orders of convergence in Table 3.3 are better than the theoretically predicted value of 0.5 (see Theorems 3.2.2 and 3.2.4).

3.3.1 Robustness: comparison of worst-case errors

It is interesting to assess the robustness of the generating vectors with respect to different weights $\boldsymbol{\gamma}$. More precisely, we would like to know how a generating vector for a particular sequence $\boldsymbol{\gamma}$ performs when applied to the space with a different set of weights. This is important for practical problems, because it is not yet well understood which weights should be chosen for a particular application.

To test this robustness, we take $n = 64007$ and take d up to 100 dimensions. For each sequence of weights $\boldsymbol{\gamma}$ from (3.17) we construct a generating vector using the fast CBC implementation of Algorithm 2. We then calculate the worst-case errors (3.11) for this generating vector for each of the five choices of weights. The results are summarised in Table 3.3.

To describe what the entries mean, recall $e_{\mathrm{pow},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$ denotes the worst-case error based on the weights $\boldsymbol{\gamma}$ and let $\boldsymbol{z}_{\boldsymbol{\gamma}}$ denote the generating vector constructed with the weights $\boldsymbol{\gamma}$. Then each entry in the table represents

$$\max_{1\le d\le 100} \frac{e_{\mathrm{pow},64007,d,\alpha,\boldsymbol{\gamma}=\mathrm{column}}(\boldsymbol{z}_{\boldsymbol{\gamma}=\mathrm{row}})}{e_{\mathrm{pow},64007,d,\alpha,\boldsymbol{\gamma}=\mathrm{column}}(\boldsymbol{z}_{\boldsymbol{\gamma}=\mathrm{column}})},$$

where the weights $\boldsymbol{\gamma}$ are specified by the headings of the rows and the columns. For example, the second entry 1.020 in the first column means

$$\max_{1\le d\le 100} \frac{e_{\mathrm{pow},64007,d,\alpha,\gamma_j=1/j^2}(\boldsymbol{z}_{\gamma_j=0.9^j})}{e_{\mathrm{pow},64007,d,\alpha,\gamma_j=1/j^2}(\boldsymbol{z}_{\gamma_j=1/j^2})} = 1.020.$$

Clearly the diagonal entries should all be 1. Since the largest entry in the table is 1.081, we conclude that the worst-case error for rules found with "incorrect" weights is never more than 8.1% larger than the worst-case error for rules found with the "correct" weights. Therefore the generating vectors obtained from our new space can be said to be reasonably robust with respect to the selection of weights.

In Table 3.4 we see a similar analysis for the unanchored Sobolev spaces. Here the worst-case errors seem to be much more sensitive to the weights $\boldsymbol{\gamma}$, in the sense that rules found with "incorrect" weights can have worst-case errors up to 78.5% larger.

	New space worst-case error ratios				
New space rules	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
Found with $\gamma_j = 1/j^2$	1	1.027	1.059	1.048	1.028
Found with $\gamma_j = 0.9^j$	1.020	1	1.047	1.006	1.002
Found with $\gamma_j = 0.05$	1.032	1.028	1	1.023	1.040
Found with $\gamma_j = 0.5$	1.039	1.007	1.044	1	1.009
Found with $\gamma_j = 0.9$	1.048	1.002	1.081	1.005	1

Table 3.3: Robustness of the generating vectors for varying weights in our new spaces

	Sobolev space worst-case error ratios				
Sobolev space rules	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
Found with $\gamma_j = 1/j^2$	1	1.208	1.545	1.253	1.267
Found with $\gamma_j = 0.9^j$	1.236	1	1.351	1.055	1.041
Found with $\gamma_j = 0.05$	1.306	1.379	1	1.334	1.462
Found with $\gamma_j = 0.5$	1.655	1.052	1.263	1	1.027
Found with $\gamma_j = 0.9$	1.785	1.058	1.389	1.066	1

Table 3.4: Robustness of the generating vectors for varying weights in the Sobolev spaces

	Sobolev space worst-case error ratios				
New space rules	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
Found with $\gamma_j = 1/j^2$	1.060	1.791	2.043	1.990	1.891
Found with $\gamma_j = 0.9^j$	1.147	1.056	1.804	1.094	1.073
Found with $\gamma_j = 0.05$	1.512	1.477	1.099	1.397	1.462
Found with $\gamma_j = 0.5$	1.495	1.063	1.256	1.052	1.081
Found with $\gamma_j = 0.9$	1.696	1.099	1.558	1.071	1.027

Table 3.5: Robustness of the generating vectors from our new spaces to Sobolev spaces

In Tables 3.5 and 3.6 we perform the same analysis as Tables 3.3 and 3.4, except that we measure the robustness to different weights and different spaces. That is, in Table 3.5 we take the generating vector constructed with a particular weight sequence in our new spaces and evaluate its worst-case error in the Sobolev spaces for different sequences $\boldsymbol{\gamma}$. Table 3.6 is the reverse of Table 3.5 in that we take the generating vectors constructed in Sobolev spaces and evaluate their worst-case errors in our new spaces for various weights. Note that the diagonal entries in these two tables no longer remain 1.

A reasonable conclusion from Table 3.6 might be that the rules found in Sobolev spaces are fairly robust for use in our new spaces. Since the CBC algorithm in our new spaces requires a significant setup cost (especially to approximate $\omega(t)$ at multiples of $1/n$), it would seem reasonable to recommend the use of rules found in Sobolev spaces. We are yet to understand the correct relationship between the weights in our new spaces and the weights in Sobolev spaces. However, since the diagonal entries in Tables 3.5 and 3.6 are in general smaller than the off-diagonal entries, a direct correspondence seems reasonably applicable in practice.

	New space worst-case error ratios				
Sobolev space rules	$\gamma_j = 1/j^2$	$\gamma_j = 0.9^j$	$\gamma_j = 0.05$	$\gamma_j = 0.5$	$\gamma_j = 0.9$
Found with $\gamma_j = 1/j^2$	1.002	1.014	1.051	1.024	1.022
Found with $\gamma_j = 0.9^j$	1.032	1.007	1.052	1.007	1.008
Found with $\gamma_j = 0.05$	1.027	1.031	1.007	1.018	1.040
Found with $\gamma_j = 0.5$	1.043	1.001	1.058	1.002	1.004
Found with $\gamma_j = 0.9$	1.065	1.007	1.081	1.009	1.008

Table 3.6: Robustness of the generating vectors from Sobolev spaces to our new spaces

3.3.2 Performance: pricing Asian options

We now examine the performance of lattice rules constructed using the fast CBC algorithm for our new spaces. To do this, we have chosen to examine the pricing of an Asian call option, as described in Section 2.7.

Recall that the payoff of an Asian option is the greater of the arithmetic average of a stock price over d equally spaced points in time less the agreed strike price K, and zero. In (2.57), we saw that the payoff can thus be formulated as

$$G(\boldsymbol{u}) = g(S(t_1), \ldots, S(t_d)) = \left(\frac{1}{d} \sum_{j=1}^{d} S(t_j) - K \right)^+. \qquad (2.57')$$

with $S(t_j)$ given by

$$S(t_j) = S_0 \exp\left((r - \tfrac{1}{2}\sigma^2) t_j + \sigma W(t_j) \right), \quad j = 1, \ldots, d$$

As we saw above, the Asian option problem is written as an integration problem

$$C = \int_{[0,1]^d} \mathrm{e}^{-rT} G(A \Phi_d^{-1}(\boldsymbol{x}))\, \mathrm{d}\boldsymbol{x}, \qquad (3.18)$$

where A is a matrix such that $AA^T = \Sigma$. In this set of experiments, we will test the problem where A is taken to be the Cholesky factor, or the PCA factor (see Section 2.7.4).

We compute the price of the Asian call option with parameters

$$S_0 = 100, \quad r = 0.1, \quad \sigma = 0.2, \quad T = 1, \quad K = 100, \quad d = 100$$

using lattice rules from our new spaces and the Sobolev spaces, and MC methods. We use both the standard construction and the PCA construction. Since all of these methods involve a degree of randomisation, we perform 10 evaluations of the integral to obtain an estimated standard error as described in Section 2.4.5. The standard errors for lattice rules with different values of n and different sequences $\boldsymbol{\gamma}$ are given in Tables 3.7–3.11. The standard errors for the MC methods are given in Table 3.12.

	Standard construction		PCA construction	
n	New space	Sobolev space	New space	Sobolev space
1009	3.23e-02	2.47e-02	6.26e-03	6.26e-03
2003	1.77e-02	1.47e-02	2.65e-03	2.54e-03
4001	5.26e-03	1.04e-02	1.30e-03	1.34e-03
8009	4.85e-03	7.56e-03	7.52e-04	8.05e-04
16001	1.57e-03	3.93e-03	4.41e-04	4.52e-04
32003	1.39e-03	1.77e-03	2.76e-04	2.67e-04
64007	1.33e-03	1.40e-03	1.00e-04	9.07e-05

Table 3.7: Comparison of standard errors for $\gamma_j = 1/j^2$

We should note immediately that the PCA construction considerably reduces the standard errors for lattice rules, but has no obvious impact on the MC approach. This is not surprising, since the PCA construction reallocates the variances to reduce the effective dimension of the problem and at the same time leaves the total variance unchanged. See [60] for a discussion of effective dimensions on finance problems.

In most cases the MC methods give the highest standard error. In fact, for the largest value of n, we see that lattice rules outperform MC methods by approximately a factor of 10 for the standard construction and a factor of 100 for the PCA construction. The choice of the sequence $\boldsymbol{\gamma}$ does not seem to have a lot of bearing on the standard error.

	Standard construction		PCA construction	
n	New space	Sobolev space	New space	Sobolev space
1009	2.04e-02	2.89e-02	6.34e-03	6.39e-03
2003	1.07e-02	1.87e-02	2.74e-03	2.66e-03
4001	7.71e-03	5.08e-03	1.20e-03	1.22e-03
8009	6.03e-03	7.18e-03	8.11e-04	8.00e-04
16001	3.45e-03	3.68e-03	4.58e-04	4.62e-04
32003	1.58e-03	2.19e-03	2.75e-04	2.78e-04
64007	1.56e-03	1.83e-03	8.48e-05	1.02e-04

Table 3.8: Comparison of standard errors for $\gamma_j = 0.9^j$

	Standard construction		PCA construction	
n	New space	Sobolev space	New space	Sobolev space
1009	1.85e-02	2.18e-02	7.12e-03	6.76e-03
2003	1.16e-02	1.72e-02	2.84e-03	3.05e-03
4001	1.02e-02	5.74e-03	1.29e-03	1.41e-03
8009	6.76e-03	3.49e-03	7.38e-04	7.97e-04
16001	3.34e-03	3.18e-03	4.61e-04	4.53e-04
32003	2.91e-03	2.03e-03	2.94e-04	2.76e-04
64007	1.44e-03	1.10e-03	1.07e-04	9.82e-05

Table 3.9: Comparison of standard errors for $\gamma_j = 0.05$

	Standard construction		PCA construction	
n	New space	Sobolev space	New space	Sobolev space
1009	3.48e-02	2.23e-02	6.05e-03	6.49e-03
2003	1.64e-02	1.75e-02	2.68e-03	2.62e-03
4001	1.03e-02	1.12e-02	1.33e-03	1.23e-03
8009	8.78e-03	6.67e-03	8.11e-04	8.15e-04
16001	4.91e-03	4.84e-03	4.92e-04	4.52e-04
32003	2.53e-03	2.13e-03	2.82e-04	2.73e-04
64007	1.84e-03	1.85e-03	9.52e-05	9.38e-05

Table 3.10: Comparison of standard errors for $\gamma_j = 0.5$

	Standard construction		PCA construction	
n	New space	Sobolev space	New space	Sobolev space
1009	2.58e-02	2.09e-02	6.43e-03	6.36e-03
2003	1.07e-02	2.04e-02	2.61e-03	2.65e-03
4001	1.05e-02	1.00e-02	1.43e-03	1.23e-03
8009	6.52e-03	4.22e-03	8.06e-04	8.17e-04
16001	6.40e-03	6.10e-03	4.81e-04	4.84e-04
32003	3.94e-03	2.42e-03	2.70e-04	2.74e-04
64007	1.42e-03	2.14e-03	9.01e-05	1.06e-04

Table 3.11: Comparison of standard errors for $\gamma_j = 0.9$

n	Standard construction	PCA construction
1009	7.76e-02	8.64e-02
2003	6.60e-02	4.91e-02
4001	7.14e-02	4.12e-02
8009	2.06e-02	3.39e-02
16001	1.83e-02	2.65e-02
32003	1.19e-02	1.10e-02
64007	1.14e-02	9.75e-03

Table 3.12: Comparison of standard errors for MC methods

There does not appear to be a clear "winner" between the new spaces and the unanchored Sobolev spaces. It should however be noted that the integrand in (3.18) does not lie in either of the spaces due to its non-smoothness: since (like most finance problems) it does not have square-integrable mixed first derivatives, it does not fall into the usual spaces where worst-case error analysis has been undertaken.

3.4 Discussion

Evidently our function spaces do not include those functions arising from option pricing because of the lack of smoothness in the integrands. Unlike those common problems in finance, many statistical problems of the form

$$I_{\rho_d}(g) = \int_{[0,1]^d} g\left(A\Phi_d^{-1}(\boldsymbol{x})\right)\,\mathrm{d}\boldsymbol{x}$$

have a function $g(\boldsymbol{u})$ which is very smooth. For example, the likelihood integral for some parameter-driven Poisson state-space models (see [6]) can be simplified in the one-dimensional case to

$$\int_{-\infty}^{\infty} \exp(yu - \mathrm{e}^u)\tfrac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{u^2}{2}}\,\mathrm{d}u, \quad y = 0, 1, \ldots.$$

The function $g(u) = \mathrm{e}^{-\mathrm{e}^u}$ (for the case $y = 0$) has infinite smoothness. However, based on our current definition of the norm, it is impossible to define a sequence

of β_k's such that both

$$\|g\|_{\mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}} = \|f\|_{H_{\mathrm{pow},1,\alpha,\gamma}} < \infty \quad \text{and} \quad \int_0^1 K_{\mathrm{pow},1,\alpha,\gamma}(x,x)\,\mathrm{d}x < \infty$$

hold; these conditions are needed to ensure that $f = g(\Phi^{-1}(\cdot)) \in H_{\mathrm{pow},1,\alpha,\gamma} \subseteq L_2([0,1])$. Note that our definition for the norm does not distinguish between positive and negative coefficients in the power-series representation of the functions. Thus if functions of the form $g(u) = \mathrm{e}^{-\lambda u^2}$ are to be included in the space, so must the functions $\mathrm{e}^{\lambda u^2}$ which are clearly not integrable.

Note that smoothness can be very misleading, because it is possible for smooth functions to have huge norms. Consider the functions of the form $f(x) = g(\Phi^{-1}(x))$ in our space $H_{\mathrm{pow},1,\alpha,\gamma}$. The norm of f in any Sobolev space with smoothness parameter 1 depends on

$$\int_0^1 [f'(x)]^2\,\mathrm{d}x = 2\pi \int_0^1 [g'(\Phi^{-1}(x))]^2 e^{[\Phi^{-1}(x)]^2}\,\mathrm{d}x = \sqrt{2\pi}\int_{-\infty}^{\infty} [g'(u)]^2 \mathrm{e}^{\frac{u^2}{2}}\,\mathrm{d}u,$$

which is clearly infinite for most $g \in H(\mathbb{R})$ or equivalently $f \in H_{\mathrm{pow},1,\alpha,\gamma}$. Thus the apparent smoothness in g does not translate to smoothness in f.

On the other hand, we can check and see if the functions $g \in \mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ actually belong to any of the Sobolev spaces in $\mathbb{R}$. In fact it can be shown that for all convergent power series $g \in \mathcal{H}_{\mathrm{pow},1,\alpha,\gamma}$ we have

$$\int_{-\infty}^{\infty} [g^{(r)}(u)]^2 \mathrm{e}^{-\alpha u^2}\,\mathrm{d}u < \infty,$$

where $\alpha \in (0, \frac{1}{2})$ is the parameter in (3.7). Results in [63] then indicate that it is possible to achieve $O(n^{-r})$ convergence with a suitable quadrature rule in one dimension. Furthermore, a Smolyak-type algorithm (linear but not equal weight) can be constructed for higher dimensions which will preserve this rate of convergence, see [62]. It is unknown whether such rate of convergence can be achieved with QMC algorithms, or in particular, with lattice rules.

Chapter 4

Randomly shifted lattice rules for unbounded integrands

In Chapter 3 we studied the problem of multivariate integration on the unit cube for unbounded integrands of the form (see (3.1) and (3.2))

$$I_{\rho_d}(g) = \int_{\mathbb{R}^d} g(\boldsymbol{u})\rho_d(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = I_d(f) \tag{4.1}$$

where

$$f(\boldsymbol{x}) = g(\Phi_d^{-1}(\boldsymbol{x})),$$

and where ρ_d is the d-dimensional normal distribution and Φ^{-1} is the cumulative inverse normal distribution. The unbounded integrands arise as a result of using the cumulative inverse normal distribution to map the integral from the unbounded domain $\mathbb{R}^d$ to the unit cube $[0,1]^d$. The function space used in Chapter 3 assumed that the functions were analytic, which is not usually the case for many finance problems, such as the ones describes in Section 2.7.

In this chapter, we expand the ideas of Chapter 3 in that we allow the probability density function ρ_d to be a more general probability density function, rather than restricting it to a Gaussian distribution (see more precise definitions below). Further, we consider a class of functions g which are only once differentiable (in each direction), as opposed to being analytic.

The work in this chapter is also an extension of [27], which proved in a *non-constructive* way that there existed QMC methods to approximate the weighted integral (4.1) for *general* ρ_d with the worst-case error of order $\mathcal{O}(n^{-1/2})$. In this chapter, we construct lattice rules which achieve this rate of convergence.

4.1 The function space

We will define the function space in the same way as in [63, 64]. We will always assume that ρ_d is a probability density function of the form

$$\rho_d(\boldsymbol{u}) = \prod_{j=1}^{d} \rho(u_j)$$

where ρ is a 1-dimensional probability density function. As before, we shall define the cumulative density function for one variable by

$$\Phi(u) = \int_{-\infty}^{u} \rho(t)\,\mathrm{d}t$$

and the d-dimensional cumulative density function by

$$\Phi(\boldsymbol{u}) = (\Phi(u_1), \ldots, \Phi(u_d))^T.$$

The corresponding inverse cumulative density functions are defined in a similar way.

We begin by noting from (4.1) that the integral can be thought of as either an integral over the space $\mathbb{R}^d$ or an integral over the d-dimensional unit cube $[0,1]^d$. Correspondingly, we will construct two spaces for the two realisations of the same integral.

Informally, the space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ will consist of function g from (4.1), while $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$ will consist of functions f of the form $f = g(\Phi_d^{-1}(\cdot))$, for $g \in \mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$.

4.1.1 The univariate case

For given $a, b \in \mathbb{R} \cup \{-\infty, \infty\}$, $a < b$, let

$$D = \overline{(a,b)} \subseteq \mathbb{R}.$$

Since we allow $a = -\infty$ and $b = \infty$, the domain can be either a closed interval $[a, b]$, a half line $[a, -\infty)$ or $(-\infty, b]$, or the whole real line $(-\infty, \infty)$. For simplicity of notation, we assume that $0 \in D$. Let $\rho : D \to \mathbb{R}_+$ be a probability density function over the domain D, i.e.,

$$\int_a^b \rho(u)\,\mathrm{d}u = 1,$$

and we consider approximating an integral of the form

$$I_\rho(g) = \int_a^b g(u)\rho(u)\,\mathrm{d}u.$$

The space $\mathcal{H}_{\mathrm{unb},1,\gamma}$

For a Lebesgue measurable and (a.e.) positive function $\psi : D \to \mathbb{R}$, let $\mathcal{H}_{\mathrm{unb},1,\gamma}$ be the space of absolutely continuous functions $g : D \to \mathbb{R}$ with derivative g' bounded in the following way

$$\|g'\psi\|^2_{L_2(D)} = \int_a^b |g'(u)\psi(u)|^2\,\mathrm{d}u < \infty.$$

This space is a separable Hilbert space when equipped with the following inner product and norm

$$\langle g, \tilde{g}\rangle_{\mathcal{H}_{\mathrm{unb},1,\gamma}} \;=\; g(0)\tilde{g}(0) + \frac{1}{\gamma}\int_a^b g'(u)\tilde{g}'(u)\psi^2(u)\,\mathrm{d}u$$

and

$$\|g\|_{\mathcal{H}_{\mathrm{unb},1,\gamma}} = \langle g, g\rangle^{1/2}_{\mathcal{H}_{\mathrm{unb},1,\gamma}}.$$

Here $\gamma > 0$ is a weight parameter. Clearly γ does not change the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$, it only changes the inner product and the norm in $\mathcal{H}_{\mathrm{unb},1,\gamma}$. As in the previous chapter, the role of γ will become apparent when we introduce the multivariate case. Notice that the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ depends on the choice of ψ. For simplicity of the notation, we shall in general not make this dependence explicit.

We assume that

$$\int_u^v \psi^{-2}(t)\,\mathrm{d}t < \infty \quad \text{for all } u, v \in D \cap (-\infty, \infty).$$

Then $\mathcal{H}_{\mathrm{unb},1,\gamma}$ is a reproducing kernel Hilbert space with the kernel $\mathcal{K}_{\mathrm{unb},1,\gamma}$ given by

$$\mathcal{K}_{\mathrm{unb},1,\gamma}(u,v) = 1 + \gamma \mathbf{1}_-(\max(u,v)) \int_{\max(u,v)}^{0} \psi^{-2}(t)\,\mathrm{d}t + \gamma \mathbf{1}_+(\min(u,v)) \int_{0}^{\min(u,v)} \psi^{-2}(t)\,\mathrm{d}t, \qquad u,v \in D. \tag{4.2}$$

Here and elsewhere, $\mathbf{1}_-$ and $\mathbf{1}_+$ denote the indicator functions of the half lines $(-\infty, 0]$ and $[0, +\infty)$, respectively.

From the definition of reproducing kernels we have

$$\mathcal{K}_{\mathrm{unb},1,\gamma}(\cdot,u) \in \mathcal{H}_{\mathrm{unb},1,\gamma} \quad \text{and } g(u) = \langle g, \mathcal{K}_{\mathrm{unb},1,\gamma}(\cdot,u)\rangle_{\mathcal{H}_{\mathrm{unb},1,\gamma}}$$

for all $u \in D$ and $g \in \mathcal{H}_{\mathrm{unb},1,\gamma}$. To see this, observe that

$$\frac{\partial}{\partial u}\mathcal{K}_{\mathrm{unb},1,\gamma}(u,v) = \begin{cases} -\gamma\psi^{-2}(u), & v < u < 0, \\ +\gamma\psi^{-2}(u), & 0 < u < v, \\ 0, & \text{otherwise.} \end{cases}$$

The significance of the weight function ψ is in the fact that by a proper choice, we could make the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ very large or very small. To see this, consider $a = -\infty$ and $b = \infty$, i.e., $D = \mathbb{R}$. By letting $\psi(u) = \exp(-\alpha u^2)$ with $\alpha > 0$, the corresponding space contains polynomials, exponential functions of the form $\exp(\beta|u|)$ for every β, and even $\exp(+\beta u^2)$ as long as $\beta < \alpha$. On the other hand, if $\psi(u)$ is bounded away from zero when $|u| \to \infty$, then among all polynomials only constant functions belong to $\mathcal{H}_{\mathrm{unb},1,\gamma}$.

The initial error $e_{0,1}(\mathcal{K}_{\mathrm{unb},1,\gamma})$ of the integration problem defined in $\mathcal{H}_{\mathrm{unb},1,\gamma}$, that is

$$e_{0,d}(\mathcal{K}_{\mathrm{unb},1,\gamma}) = \sup_{\substack{g \in \mathcal{H}_{\mathrm{unb},1,\gamma} \\ \|g\|_{\mathcal{H}_{\mathrm{unb},1,\gamma}} \le 1}} |I_\rho(g)| = \left(\int_a^b \int_a^b \mathcal{K}_{\mathrm{unb},1,\gamma}(u,v)\rho(u)\rho(v)\,\mathrm{d}u\,\mathrm{d}v \right)^{1/2}.$$

For the problem to be well defined we have to assume that $e_{0,1}(\mathcal{K}_{\mathrm{unb},1,\gamma})$ is finite. From (4.2) it can be shown that this assumption is equivalent to

$$C_0 = \int_a^0 \psi^{-2}(t) \left(\int_a^t \rho(u)\,\mathrm{d}u \right)^2 \mathrm{d}t + \int_0^b \psi^{-2}(t) \left(\int_t^b \rho(u)\,\mathrm{d}u \right)^2 \mathrm{d}t < \infty, \tag{4.3}$$

and we have $e_{0,1}(\mathcal{K}_{\mathrm{unb},1,\gamma}) = (1 + C_0\gamma)^{1/2}$. Furthermore, we assume an even stronger condition

$$\int_a^b \mathcal{K}_{\mathrm{unb},1,\gamma}(u,u)\rho(u)\,\mathrm{d}u < \infty,$$

which ensures that the embedding of $\mathcal{H}_{\mathrm{unb},1,\gamma}$ is in $L_{2,\rho}(D)$. Again it follows from (4.2) that we require

$$C_1 = \int_a^0 \psi^{-2}(t) \int_a^t \rho(u)\,\mathrm{d}u\,\mathrm{d}t + \int_0^b \psi^{-2}(t) \int_t^b \rho(u)\,\mathrm{d}u\,\mathrm{d}t < \infty. \tag{4.4}$$

Clearly we have $C_1 \geq C_0$ for all choices of ψ and ρ.

Example 4.1.1 Consider $D = \mathbb{R}$ and a Gaussian distribution

$$\rho(u) = \frac{\exp(-u^2/(2\lambda))}{\sqrt{2\pi\lambda}}, \quad \lambda > 0.$$

Using

$$\frac{1}{t}\left(1 - \frac{1}{t^2}\right)\mathrm{e}^{-t^2/2} \leq \frac{1}{\sqrt{2\pi}} \int_t^\infty \mathrm{e}^{-u^2/2}\,\mathrm{d}u \leq \frac{1}{t}\mathrm{e}^{-t^2/2} \quad \text{for all } t > 0,$$

we see that both (4.3) and (4.4) hold if $\psi(u)$ converges to zero (with $|u| \to \infty$) slower than any Gaussian density. If we take $\psi(u) = \exp(-|u|/\alpha)$, then (4.3) and (4.4) hold for all $\alpha > 0$, and the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ contains functions such as $\exp(|u|/\beta)$ provided that $\beta > \alpha$. If we take $\psi(u) = \exp(-u^2/(2\alpha))$, then it is easy to see that (4.3) holds if and only if $\alpha > \lambda$ and (4.4) holds if and only if $\alpha > 2\lambda$. Moreover, the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ contains even such fast diverging functions as $\exp(+u^2/(2\beta))$ as long as $\beta > \alpha$.

Example 4.1.2 Consider $D = [a, \infty)$ for finite $a \leq 0$ and an exponential distribution

$$\rho(u) = \frac{\exp(-(u-a)/\lambda)}{\lambda}, \quad \lambda > 0.$$

If $\psi(u)$ converges to zero slower than any function with an exponential decay then (4.3) and (4.4) are satisfied. Consider therefore $\psi(u) = \exp(-u/\alpha)$. Then 4.3 holds if and only if $\alpha > \lambda$ and 4.4 holds if and only if $\alpha > 2\lambda$. Clearly in this case the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ contains functions such as $\exp(+u/\beta)$ if $\beta > \alpha$.

Example 4.1.3 Consider $D = \mathbb{R}$ and a two-tailed exponential distribution

$$\rho(u) = \frac{\exp(-|u|/\lambda)}{2\lambda}, \quad \lambda > 0.$$

Taking $\psi(u) = \exp(-|u|/\alpha)$ we see that (4.3) holds if and only if $\alpha > \lambda$ and (4.4) holds if and only if $\alpha > 2\lambda$. With this choice of ψ, the space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ contains functions such as $\exp(|u|/\beta)$ provided that $\beta > \alpha$.

Example 4.1.4 Consider $D = \mathbb{R}$ and a logistic distribution

$$\rho(u) = \frac{1}{\lambda} \frac{\mathrm{e}^{u/\lambda}}{(1 + \mathrm{e}^{u/\lambda})^2}, \quad \lambda > 0.$$

This density function has a bell shape similar to Gaussian, but its tails have exponential decay, since

$$\frac{1}{4} e^{-|u|/\lambda} \leq \frac{\mathrm{e}^{u/\lambda}}{(1 + \mathrm{e}^{u/\lambda})^2} \leq \mathrm{e}^{-|u|/\lambda}.$$

Suppose that $\psi(u) = \mathrm{e}^{u/\alpha}/(1 + \mathrm{e}^{u/\alpha})^2$. Then it is not hard to see that (4.3) holds if and only if $\alpha > \lambda$ and (4.4) holds if and only if $\alpha > 2\lambda$. This choice of ψ leads to a space $\mathcal{H}_{\mathrm{unb},1,\gamma}$ containing functions such as $\exp(|u|/\beta)$ provided that $\beta > \alpha$.

Example 4.1.5 Consider $D = \mathbb{R}$ and

$$\rho(u) = \frac{\lambda - 1}{2} \frac{1}{(1 + |u|)^\lambda}, \quad \lambda > 1.$$

Suppose also that $\psi(u) = (1+|u|)^{-\alpha}$. Then (4.3) holds if and only if $\alpha < \lambda - 3/2$ and (4.4) holds if and only if $\alpha < \lambda/2 - 1$. Clearly now $\mathcal{H}_{\mathrm{unb},1,\gamma}$ contains polynomials of degree smaller than $\alpha + 1/2$.

The space $H_{\mathrm{unb},1,\gamma}$

Let Φ^{-1} be the inverse of the cumulative density function

$$\Phi(u) = \int_a^u \rho(t)\, \mathrm{d}t.$$

Then after the change of variables $x = \Phi(u)$, as discussed above, we have

$$\int_a^b g(u)\rho(u)\,\mathrm{d}u = \int_0^1 f(x)\,\mathrm{d}x \quad \text{where } f(x) = g(\Phi^{-1}(x)).$$

Let $H_{\mathrm{unb},1,\gamma}$ denote the corresponding space of functions $f = g(\Phi^{-1}(\cdot))$ defined over the domain $[0,1]$. The space $H_{\mathrm{unb},1,\gamma}$ is isometric to $\mathcal{H}_{\mathrm{unb},1,\gamma}$ defined earlier

$$g \in \mathcal{H}_{\mathrm{unb},1,\gamma} \iff f = g(\Phi^{-1}(\cdot)) \in H_{\mathrm{unb},1,\gamma} \quad \text{and } \|g\|_{\mathcal{H}_{\mathrm{unb},1,\gamma}} = \|f\|_{H_{\mathrm{unb},1,\gamma}}.$$

Similarly, we see that $H_{\mathrm{unb},1,\gamma}$ is a reproducing kernel Hilbert space with the kernel given by

$$K_{\mathrm{unb},1,\gamma}(x,y) = \mathcal{K}_{\mathrm{unb},1,\gamma}(\Phi^{-1}(x), \Phi^{-1}(y)), \quad x, y \in [0,1].$$

Note that we use calligraphic letters for the space defined over the general D in contrast to upright letters for the space defined over the unit interval $[0,1]$. (Technically, the domain of $H_{\mathrm{unb},1,\gamma}$ could be either $[0,1]$, $(0,1]$, $[0,1)$ or $(0,1)$, depending on whether the domain D of $\mathcal{H}_{\mathrm{unb},1,\gamma}$ is a closed interval, a half line, or the whole real line.) The space $H_{\mathrm{unb},1,\gamma}$ depends on the choice of ψ. So as to ease the congestion in the notation, we will not include the ψ in the subscripts.

Since

$$\begin{aligned}
e_{0,1}(K_{\mathrm{unb},1,\gamma}) &= \left(\int_0^1\int_0^1 K_{\mathrm{unb},1,\gamma}(x,y)\,\mathrm{d}x\,\mathrm{d}y\right)^{1/2} \\
&= \left(\int_a^b\int_a^b K_{\mathrm{unb},1,\gamma}(\Phi(u),\Phi(v))\rho(u)\rho(v)\,\mathrm{d}u\,\mathrm{d}v\right)^{1/2} \\
&= \left(\int_a^b\int_a^b \mathcal{K}_{\mathrm{unb},1,\gamma}(u,v)\rho(u)\rho(v)\,\mathrm{d}u\,\mathrm{d}v\right)^{1/2} \\
&= (1+C_0\gamma)^{1/2} = e_{0,1}(\mathcal{K}_{\mathrm{unb},1,\gamma}),
\end{aligned}$$

the condition (4.3) guarantees that every function f from $H_{\mathrm{unb},1,\gamma}$ is integrable.

Moreover, we have for all $f \in H_{\mathrm{unb},1,\gamma}$ that

$$\begin{aligned}
\|f\|_{L_2([0,1])} &= \left(\int_0^1 |f(x)|^2 \, \mathrm{d}x \right)^{1/2} \\
&\leq \left(\int_0^1 K_{\mathrm{unb},1,\gamma}(x,x) \, \mathrm{d}x \right)^{1/2} \|f\|_{H_{\mathrm{unb},1,\gamma}} \\
&= \left(\int_a^b \mathcal{K}_{\mathrm{unb},1,\gamma}(u,u) \, \mathrm{d}u \right)^{1/2} \|f\|_{H_{\mathrm{unb},1,\gamma}} \\
&= (1 + C_1\gamma)^{1/2} \|f\|_{H_{\mathrm{unb},1,\gamma}} .
\end{aligned}$$

Hence the condition (4.4) implies that $H_{\mathrm{unb},1,\gamma}$ is embedded in $L_2([0,1])$, and all functions f in $H_{\mathrm{unb},1,\gamma}$ are square-integrable.

We end this section with a discussion on the shift-invariant kernel (see Section 2.3.2) associated with $K_{\mathrm{unb},1,\gamma}$, which is defined by

$$K^{\mathrm{sh}}_{\mathrm{unb},1,\gamma}(x,y) = \int_0^1 K_{\mathrm{unb},1,\gamma}(\{x+\Delta\},\{y+\Delta\}) \, \mathrm{d}\Delta, \quad x,y \in [0,1].$$

From this definition, it is not hard to see that $K^{\mathrm{sh}}_{\mathrm{unb},1,\gamma}$ depends only on $\{x-y\}$. Here is the derivation of $K^{\mathrm{sh}}_{\mathrm{unb},1,\gamma}(x,y)$ together with some properties that will be needed later.

Lemma 4.1.6 *The shift-invariant kernel associated with $K_{\mathrm{unb},1,\gamma}$ is of the form*

$$K^{\mathrm{sh}}_{\mathrm{unb},1,\gamma}(x,y) = 1 + \gamma\omega(\{x-y\}), \quad x,y \in [0,1],$$

where $\omega(t) = \Upsilon(t) + \Upsilon(1-t)$, with

$$\Upsilon(t) = \int_{\Phi^{-1}(t)}^0 \psi^{-2}(u)(\Phi(u) - t) \, \mathrm{d}u. \tag{4.5}$$

Moreover, ω is non-negative, symmetric along $t = 1/2$, with

$$\omega(0) = C_1, \quad \int_0^1 \omega(t) \, \mathrm{d}t = C_0, \quad \text{and } \omega''(t) \geq 0 \quad \text{for all } t \in (0,1),$$

where C_0 and C_1 are as defined in (4.3) and (4.4).

Proof. Clearly $K^{\mathrm{sh}}_{\mathrm{unb},1,\gamma}(x,y) = 1 + \gamma\omega(\{x-y\})$ with $\omega(t) = \omega_1(t) + \omega_2(t)$, for

$$\begin{aligned}
\omega_1(t) &= \int_0^1 \mathbf{1}_-(\max(\Phi^{-1}(\Delta), \Phi^{-1}(\{\Delta+t\}))) \int_{\overline{m}(\Delta,t)}^0 \psi^{-2}(u) \, \mathrm{d}u \, \mathrm{d}\Delta, \\
\omega_2(t) &= \int_0^1 \mathbf{1}_+(\min(\Phi^{-1}(\Delta), \Phi^{-1}(\{\Delta+t\}))) \int_0^{\underline{m}(\Delta,t)} \psi^{-2}(u) \, \mathrm{d}u \, \mathrm{d}\Delta,
\end{aligned}$$

where

$$\underline{m}(\Delta, t) = \min(\Phi^{-1}(\Delta), \Phi^{-1}(\{\Delta + t\}))$$
$$\overline{m}(\Delta, t) = \max(\Phi^{-1}(\Delta), \Phi^{-1}(\{\Delta + t\})).$$

Consider first $\omega_1(t)$. Since Φ^{-1} is monotonically increasing, $\overline{m}(\Delta, t)$ equals $\Phi^{-1}(\max(\Delta, \{\Delta + t\}))$, which equals $\Phi^{-1}(\Delta + t)$ when $\Delta \leq 1 - t$ and equals $\Phi^{-1}(\Delta)$ when $\Delta \geq 1 - t$. Thus

$$\begin{aligned}
\omega_1(t) &= \int_0^{1-t} \mathbf{1}_-(\Phi^{-1}(\Delta + t)) \int_{\Phi^{-1}(\Delta+t)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}\Delta \\
&\quad + \int_{1-t}^1 \mathbf{1}_-(\Phi^{-1}(\Delta)) \int_{\Phi^{-1}(\Delta)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}\Delta \\
&= \int_t^1 \mathbf{1}_-(\Phi^{-1}(z)) \int_{\Phi^{-1}(z)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}z \\
&\quad + \int_{1-t}^1 \mathbf{1}_-(\Phi^{-1}(\Delta)) \int_{\Phi^{-1}(\Delta)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}\Delta.
\end{aligned}$$

Let $\alpha_0 = \Phi(0)$. Since $\Phi^{-1}(z) \leq 0$ iff $z \leq \alpha_0$, we have

$$\begin{aligned}
\omega_1(t) &= \mathbf{1}_+(\alpha_0 - t) \int_t^{\alpha_0} \int_{\Phi^{-1}(z)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}z \\
&\quad + \mathbf{1}_+(\alpha_0 - 1 + t) \int_{1-t}^{\alpha_0} \int_{\Phi^{-1}(\Delta)}^0 \psi^{-2}(u)\,\mathrm{d}u\,\mathrm{d}\Delta \\
&= \mathbf{1}_+(\alpha_0 - t) \int_{\Phi^{-1}(t)}^0 \psi^{-2}(u)(\Phi(u) - t)\,\mathrm{d}u \\
&\quad + \mathbf{1}_+(\alpha_0 - 1 + t) \int_{\Phi^{-1}(1-t)}^0 \psi^{-2}(u)(\Phi(u) - 1 + t)\,\mathrm{d}u.
\end{aligned}$$

Similarly, one can show that

$$\begin{aligned}
\omega_2(t) &= \mathbf{1}_+(1 - t - \alpha_0) \int_0^{\Phi^{-1}(1-t)} \psi^{-2}(u)(1 - t - \Phi(u))\,\mathrm{d}u \\
&\quad + \mathbf{1}_+(t - \alpha_0) \int_0^{\Phi^{-1}(t)} \psi^{-2}(u)(t - \Phi(u))\,\mathrm{d}u.
\end{aligned}$$

Hence we have $\omega(t) = \Upsilon(t) + \Upsilon(1 - t)$, with

$$\Upsilon(t) = \int_{\Phi^{-1}(t)}^0 \psi^{-2}(u)(\Phi(u) - t)\,\mathrm{d}u.$$

It is easy to show that

$$\Upsilon'(t) = -\int_{\Phi^{-1}(t)}^{0} \psi^{-2}(u)\,\mathrm{d}u, \quad \Upsilon''(t) = \frac{\psi^{-2}(\Phi^{-1}(t))}{\rho(\Phi^{-1}(t))},$$

and

$$\begin{aligned}\int_0^1 \Upsilon(t)\,\mathrm{d}t &= \int_0^{\alpha_0}\int_{\Phi^{-1}(t)}^{0} \psi^{-2}(u)(\Phi(u)-t)\,\mathrm{d}u\,\mathrm{d}t \\ &\quad + \int_{\alpha_0}^1\int_0^{\Phi^{-1}(t)} \psi^{-2}(u)(t-\Phi(u))\,\mathrm{d}u\,\mathrm{d}t \\ &= \int_a^0 \psi^{-2}(u)\frac{(\Phi(u))^2}{2}\,\mathrm{d}u + \int_0^b \psi^{-2}(u)\frac{(1-\Phi(u))^2}{2}\,\mathrm{d}u.\end{aligned}$$

Thus

$$\begin{aligned}&\omega(0) = \Upsilon(0)+\Upsilon(1) = \int_a^0 \psi^{-2}(u)\Phi(u)\,\mathrm{d}u + \int_0^b \psi^{-2}(u)(1-\Phi(u))\,\mathrm{d}u = C_1, \\ &\int_0^1 \omega(t)\,\mathrm{d}t = 2\int_0^1 \Upsilon(t)\,\mathrm{d}t = C_0, \\ &\omega''(t) = \Upsilon''(t)+\Upsilon''(1-t) = \frac{\psi^{-2}(\Phi^{-1}(t))}{\rho(\Phi^{-1}(t))} + \frac{\psi^{-2}(\Phi^{-1}(1-t))}{\rho(\Phi^{-1}(1-t))} \geq 0 \quad \forall t.\end{aligned}$$

This completes the proof. □

4.1.2 The multivariate case

For $d \geq 2$, we study d-dimensional integrals of the form

$$\int_{D^d} g(\boldsymbol{u})\,\rho_d(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}, \quad \text{where } \rho_d(\boldsymbol{u}) = \prod_{j=1}^{d}\rho(u_j).$$

We now define the spaces of d-variate functions as tensor products of the spaces $\mathcal{H}_{\mathrm{unb},1,\gamma}$ and $H_{\mathrm{unb},1,\gamma}$.

The space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$

For a given sequence of non-increasing positive weights $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$, we define the reproducing kernel $\mathcal{K}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ as the tensor product of the kernels $\mathcal{K}_{\mathrm{unb},1,\gamma_j}$,

$$\mathcal{K}_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{u},\boldsymbol{v}) = \prod_{j=1}^{d}\mathcal{K}_{\mathrm{unb},1,\gamma_j}(u_j,v_j), \quad \boldsymbol{u},\boldsymbol{v}\in D^d.$$

The space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ is then the Hilbert space generated by the one-dimensional reproducing kernel $\mathcal{K}_{\mathrm{unb},d,\boldsymbol{\gamma}}$.

Alternatively, the space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ can be characterised in terms of its inner product

$$\langle g, \tilde{g} \rangle_{\mathcal{H}_{\mathrm{unb},d,\gamma}} = g(\mathbf{0})\tilde{g}(\mathbf{0}) + \sum_{\emptyset \neq \mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}}^{-1} \int_{D^{|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{u}_{\mathfrak{u}}} g(\boldsymbol{u}_{\mathfrak{u}}, \mathbf{0}) \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{u}_{\mathfrak{u}}} \tilde{g}(\boldsymbol{u}_{\mathfrak{u}}, \mathbf{0}) \, \psi_{\mathfrak{u}}^2(\boldsymbol{u}_{\mathfrak{u}}) \, \mathrm{d}\boldsymbol{u}_{\mathfrak{u}},$$

where $\mathfrak{u}$ is defined as in Section 2.4.1. By $(\boldsymbol{x}_{\mathfrak{u}}, \mathbf{0})$ we mean a d-dimensional vector whose jth coordinate is x_j if $j \in \mathfrak{u}$ and zero otherwise. Moreover,

$$\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j \quad \text{and } \psi_{\mathfrak{u}}(\boldsymbol{u}_{\mathfrak{u}}) = \prod_{j \in \mathfrak{u}} \psi(u_j).$$

Letting

$$\left(\bigotimes_{j=1}^{d} g_j \right)(\boldsymbol{u}) = \prod_{j=1}^{d} g_j(x_j),$$

the space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ is the completion of

$$\operatorname{span} \left\{ \bigotimes_{j=1}^{d} g_j : g_j \in \mathcal{H}_{\mathrm{unb},1,\gamma_j} \right\},$$

with respect to the norm $\|\cdot\|_{\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}} = \langle \cdot, \cdot \rangle_{\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}}^{1/2}$.

The space $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$

Similarly to the one-dimensional case, we will now define the corresponding space $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$ over $[0,1]^d$ which is isometric to $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$. Again we use upright and calligraphic letters to make a distinction between these two spaces. Using the substitution $\boldsymbol{x} = \Phi_d(\boldsymbol{u}) = (\Phi(u_1), \ldots, \Phi(u_d))^T$, we have

$$\int_{D^d} g(\boldsymbol{u}) \rho_d(\boldsymbol{u}) \, \mathrm{d}\boldsymbol{u} = \int_{[0,1]^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \quad \text{with } f(\boldsymbol{x}) = g(\Phi_d^{-1}(\boldsymbol{x})).$$

The space $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$, which contains the corresponding functions $f = g(\Phi^{-1}(\cdot))$, is isometric to $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$, that is,

$$g \in \mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}} \iff f = g(\Phi_d^{-1}(\cdot)) \in H_{\mathrm{unb},d,\boldsymbol{\gamma}} \quad \text{and } \|g\|_{\mathcal{H}_{\mathrm{unb},d,\gamma}} = \|f\|_{H_{\mathrm{unb},d,\gamma}}.$$

The reproducing kernel in $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$ is given by

$$\begin{aligned} K_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) &= \mathcal{K}_{\mathrm{unb},d,\boldsymbol{\gamma}}(\Phi_d^{-1}(\boldsymbol{x}),\Phi_d^{-1}(\boldsymbol{y})) \\ &= \prod_{j=1}^{d} \mathcal{K}_{\mathrm{unb},1,\gamma_j}(\Phi^{-1}(x_j),\Phi^{-1}(y_j)), \quad \boldsymbol{x},\boldsymbol{y}\in[0,1]^d, \end{aligned}$$

with the associated shift-invariant kernel

$$\begin{aligned} K^{\mathrm{sh}}_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) &= \prod_{j=1}^{d} K_{\mathrm{unb},1,\gamma_j}(x_j,y_j) \\ &= \prod_{j=1}^{d} \left(1+\gamma_j\omega(\{x_j-y_j\})\right), \quad \boldsymbol{x},\boldsymbol{y}\in[0,1]^d. \end{aligned}$$

QMC methods are traditionally designed for integrals over the unit cube. That is, we construct a set of points $P_{n,d}=\{\boldsymbol{t}_0,\boldsymbol{t}_1,\ldots,\boldsymbol{t}_{n-1}\}$ with each point lying in the unit cube. For an integral such as $I_{\rho_d}(g)$ in (4.1) defined over $\mathbb{R}^d$, we desire to find a point set $\boldsymbol{\tau}_0,\boldsymbol{\tau}_1,\ldots,\boldsymbol{\tau}_{n-1}$ where $\boldsymbol{\tau}_k=\Phi_d^{-1}(\boldsymbol{t}_k)$ for some $\boldsymbol{t}_k\in(0,1)^d$, for $k=0,1,\ldots,n-1$.

We shall carry out our analysis in the space $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$ to construct the point set for the integration problem $I_d(f)$ and then exploit the isometry between $H_{\mathrm{unb},d,\boldsymbol{\gamma}}$ and $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ to construct the point set for $I_{\rho_d}(g)$.

4.2 Worst-case error analysis

From the theory developed in Section 2.3.2, the squared worst-case error for a point set $P_{n,d}=\{\boldsymbol{t}_0,\boldsymbol{t}_1,\ldots,\boldsymbol{t}_{n-1}\}$ of points in the unit cube is given by

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

By $M_{\mathrm{unb},n,d,\boldsymbol{\gamma}}$ we denote the QMC mean for this space. As stated in Section 2.3.3, the QMC mean is defined as the root mean squared QMC worst-case

error over all possible points $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1} \in [0,1]^d$. We have

$$\begin{aligned} M^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}} &= \int_{[0,1]^{nd}} e^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}) \,\mathrm{d}\boldsymbol{t}_0 \,\mathrm{d}\boldsymbol{t}_1 \cdots \mathrm{d}\boldsymbol{t}_{n-1} \\ &= \frac{1}{n}\left(\int_{[0,1]^d} K_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} - \int_{[0,1]^{2d}} K_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y}\right) \\ &= \frac{1}{n}\left(\prod_{j=1}^{d}(1+C_1\gamma_j) - \prod_{j=1}^{d}(1+C_0\gamma_j)\right). \end{aligned}$$

By the averaging argument, there clearly exists a set of points $\{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ such that

$$e_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(P_{n,d}; K_{\mathrm{unb},d,\boldsymbol{\gamma}}) \le M_{\mathrm{unb},n,d,\boldsymbol{\gamma}} \le \frac{1}{\sqrt{n}} \exp\left(\frac{C_1}{2}\sum_{j=1}^{d}\gamma_j\right).$$

This leads to a $\mathcal{O}(n^{-1/2})$ rate of convergence. Moreover, the implied constant can be bounded independent of d provided that $\sum_{j=1}^{\infty}\gamma_j < \infty$. We shall use the QMC mean as a benchmark for our lattice rules below.

We now calculate the expected worst-case error for a randomly-shifted lattice rule with generating vector $\boldsymbol{z}$. As in Section 3.2, we will refer to the worst-case error for a lattice rule with generating vector $\boldsymbol{z}$ and shift $\boldsymbol{\Delta}$ as $e_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z},\boldsymbol{\Delta})$. If the shift is chosen randomly, we shall refer to the expected randomly-shifted worst-case error as $e_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z})$.

Following Theorem 2.3.3, we can write the squared worst-case error for a randomly shifted lattice rule as

$$\begin{aligned} e^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}) &= \int_{[0,1]^d} e^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z},\boldsymbol{\Delta}) \,\mathrm{d}\boldsymbol{\Delta} \\ &= -\int_{[0,1]^{2d}} K_{\mathrm{unb},d,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y} + \frac{1}{n}\sum_{i=0}^{n-1} K^{\mathrm{sh}}_{\mathrm{unb},d,\boldsymbol{\gamma}}\left(\left\{\tfrac{i\boldsymbol{z}}{n}\right\}, \boldsymbol{0}\right) \\ &= -\prod_{j=1}^{d}(1+C_0\gamma_j) + \frac{1}{n}\sum_{i=0}^{n-1}\prod_{j=1}^{d}\left(1+\gamma_j\omega\left(\left\{\tfrac{iz_j}{n}\right\}\right)\right), \end{aligned} \tag{4.6}$$

Therefore, we know there must exist at least one shift $\boldsymbol{\Delta}$ such that

$$e^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z},\boldsymbol{\Delta}) \le e^2_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}).$$

In other words, it serves as an upper bound for the worst-case error of shifted rank-1 lattice rules with deterministic shifts.

We see from Lemma 4.1.6 that

$$\omega(0) = C_1, \quad \int_0^1 \omega(t)\,\mathrm{d}t = C_0, \quad \text{and } \omega''(t) \geq 0 \quad \text{for all } t \in (0,1).$$

The fact that ω is convex and symmetric about $t = 1/2$ implies that for $n = p^m$ the power of a prime p (see Lemma 3.2.1)

$$\frac{1}{\phi(p^m)} \sum_{z \in \mathcal{Z}_{p,m}} \omega\left(\frac{z}{p^m}\right) < \int_0^1 \omega(t)\,\mathrm{d}t = C_0 \tag{4.7}$$

which is an essential step for our analysis below.

We now use a component-by-component (CBC) algorithm to construct the generating vector $\boldsymbol{z}$. The vector $\boldsymbol{z}$ constructed this way has a worst case error not greater than the QMC mean.

Algorithm 3 CBC algorithm for the space of unbounded functions

Require: Let $n = p^m$ be the power of a prime p, $d_{\max}$ some integer and ψ some function such that $g \in \mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ or equivalently $f \in H_{\mathrm{unb},d,\boldsymbol{\gamma}}$

1: Set $z_1^* = 1$
2: **for** $d = 1$ to $d_{\max} - 1$ **do**
3: Find $z_{d+1}^* \in \mathcal{Z}_{p,m}$ which minimises $e_{\mathrm{unb},p^m,d+1,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))$
4: Set $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$
5: **end for**

Theorem 4.2.1 *For $n = p^m$ the power of a prime p, then the generating vector $\boldsymbol{z}_d^* = (z_1^*, \ldots, z_d^*) \in \mathcal{Z}_{p,m}^d$ constructed by Algorithm 3 satisfies*

$$e_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(z_1^*, \ldots, z_d^*) < M_{\mathrm{unb},n,d,\boldsymbol{\gamma}}$$

for all $d = 1, 2, \ldots, d_{\max}$.

Proof. The proof is very similar to the proof of Theorem 3.2.5 and is excluded here for the sake of brevity. □

In the implementation of Algorithm 3 we once again use a modified version of the fast CBC algorithm of Cools and Nuyens mentioned above. This allows

us to calculate the vector $\boldsymbol{z}^*$ in $\mathcal{O}(dn \log n)$ operations. The function ω must be pre-computed at all multiples of $1/n$. This requires $\mathcal{O}(n)$ storage.

Finally, we can easily calculate a lower bound for the worst-case error. As was the case for the space $H_{\text{pow},d,\alpha,\boldsymbol{\gamma}}$, we use the fact that ω is non-negative and dropping the terms in (4.6) where $i \neq 0$, we obtain

$$e^2_{\text{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z}) \geq -\prod_{j=1}^{d}(1 + C_0\gamma_j) + \frac{1}{n}\prod_{j=1}^{d}(1 + C_1\gamma_j) \quad \text{for all } \boldsymbol{z} \in \mathcal{Z}^d_{n,1}.$$

Using this as lower bound and the QMC mean $M_{\text{unb},n,d,\boldsymbol{\gamma}}$ as upper bound, it follows that the condition $\sum_{j=1}^{\infty}\gamma_j < \infty$ is both necessary and sufficient for $e_{\text{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z})$ to be bounded independently of d.

4.3 Numerical experiments

In this section, we test the performance of the randomly-shifted lattice rules generated by Algorithm 3. We test the lattice rules with the same problem which we used for the analytic space of functions in Section 3.3.2, namely the Asian option pricing problem, with the same values for the parameters.

We have seen in Section 3.3.2 that the PCA construction gives far superior performance to the standard construction. For this reason, we will only include results in this section using the PCA construction.

Therefore, we are solving the problem over $\mathbb{R}^d$ of

$$C = \int_{\mathbb{R}^d} g(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}, \quad \text{where } g(\boldsymbol{u}) = \frac{\mathrm{e}^{-rT}}{(\sqrt{2\pi})^d\sqrt{\det\Sigma}}G(\boldsymbol{u})\exp\left(\tfrac{1}{2}\boldsymbol{u}^T\Sigma^{-1}\boldsymbol{u}\right) \quad (4.8)$$

or equivalently over the unit cube

$$C = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \quad \text{where } f(\boldsymbol{x}) = \mathrm{e}^{-rT}G(A\Phi_d^{-1}(\boldsymbol{x})), \quad (4.9)$$

where G is the payoff function as defined in (2.57), Σ is the covariance matrix as defined in (2.56), A is the matrix with columns as defined in (2.61) and Φ^{-1} is the inverse cumulative normal density function.

Thus the density ρ is pre-determined, but we have the freedom to choose the weight function ψ. We must stress at this point that, no matter how we choose ψ, the function space $\mathcal{H}_{\mathrm{unb},d,\boldsymbol{\gamma}}$ will not include this function g. Nevertheless, we will ignore this fact and proceed to choose ψ to capture some features of g. A closer examination of the payoff function indicates that, at least in one dimension, g behaves like $\exp(\sigma u)$ when $|u| \to \infty$. Thus we shall choose ψ so that (4.3) and (4.4) both hold with respect to a Gaussian ρ, and we want $\mathcal{H}_{\mathrm{unb},1,\gamma}$ to include the function $\exp(\sigma u)$. Three possibilities are:

1. Gaussian	$\psi(u) = \exp\left(-\frac{u^2}{2\alpha}\right),$	$\alpha > 2.$
2. Two-tailed exponential	$\psi(u) = \exp\left(-\frac{\lvert u\rvert}{\alpha}\right),$	$0 < \alpha < 1/\sigma.$
3. Logistic	$\psi(u) = \dfrac{\mathrm{e}^{u/\alpha}}{(1+\mathrm{e}^{u/\alpha})^2},$	$0 < \alpha < 1/\sigma.$

See Examples 4.1.1, 4.1.3, and 4.1.4 for a discussion of these choices. Note that in order to calculate the worst case error, we must evaluate the function ω, or equivalently, the function Υ given in (4.5), at multiples of $1/n$. In this case Φ is the cumulative normal distribution function, which can be evaluated with any standard computational package. The integral in Υ can be evaluated using a one-dimensional quadrature formula. The values of C_0 and C_1 may be calculated in a similar fashion.

Remark 4.3.1 It is not entirely true that the density ρ is fixed in this case. It is always possible to write

$$\int_{[0,1]^d} g(\boldsymbol{u})\rho_d(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = \int_{[0,1]^d} \frac{g(\boldsymbol{u})\rho_d(\boldsymbol{u})}{\widetilde{\rho}_d(\boldsymbol{u})}\widetilde{\rho}_d(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u},$$

where $\widetilde{\rho}_d$ can be the product of any univariate probability density. By using a different density, we can change the feature of the transformed integrand, making it bounded or unbounded near the boundary of the cube. Consider for example the one dimensional integral

$$\int_{-\infty}^{\infty} \exp(\sigma u)\frac{\mathrm{e}^{-u^2/2}}{\sqrt{2\pi}}\,\mathrm{d}\boldsymbol{x}.$$

When ρ is the standard normal density, the transformed integrand in the unit interval is $\exp(\sigma\Phi^{-1}(x))$, which is clearly unbounded at $x = 1$. If we take instead $\widetilde{\rho}(u) = \mathrm{e}^u/(1+\mathrm{e}^u)^2$, then the transformed integrand is

$$\exp(\sigma\widetilde{\Phi}^{-1}(x))\frac{\mathrm{e}^{-[\widetilde{\Phi}^{-1}(x)]^2/2}}{\sqrt{2\pi}}\frac{(1+\mathrm{e}^{\widetilde{\Phi}^{-1}(x)})^2}{\mathrm{e}^{\widetilde{\Phi}^{-1}(x)}}, \quad \text{with } \widetilde{\Phi}^{-1}(x) = \log\left(\tfrac{x}{1-x}\right),$$

which is bounded on the entire interval $[0,1]$. The question we should ask ourselves is whether it is better to work with an unbounded integrand arising from the natural transformation, or is it better to seek a transformation which ensures that the transformed integrand is bounded? This falls outside the scope of the thesis. But it is our opinion that an unbounded integrand with weak singularities is easier to handle in practice than a bounded integrand with huge norms resulting from the large derivative values near the boundary.

We consider three cases: for a Gaussian ψ we take $\alpha = 5$; for a two-tailed exponential ψ we take $\alpha = 2$; and for a logistic ψ we take $\alpha = 2$ as well. In each case, we carry out the fast CBC algorithm with $d = 100$ and prime numbers $n = 1009$, 2003, 4001, 8009, 16001, 32003, and 64007, using three different "styles" of weights:

$$\gamma_j \propto 1/j^2 \text{ (slow decaying)}, \quad \gamma_j \propto 0.9^j \text{ (fast decaying)}, \quad \text{and} \quad \gamma_j \propto 1 \text{ (equal)}.$$

Note that each of the three cases corresponds to a different function space, with different values of C_0, C_1, and initial error $e_{\mathrm{unb},0,d,\boldsymbol{\gamma}}$. Clearly we cannot directly compare the worst-case errors. It follows from the upper and lower bounds in the previous section that the normalised worstcase error satisfies

$$\sqrt{\max\left(\frac{R}{n}-1,0\right)} \le \frac{e_{\mathrm{unb},n,d,\boldsymbol{\gamma}}(\boldsymbol{z})}{e_{\mathrm{unb},0,d,\boldsymbol{\gamma}}} \le \sqrt{\frac{R-1}{n}},$$

where

$$R = \prod_{j=1}^{d}\frac{1+C_1\gamma_j}{1+C_0\gamma_j}.$$

Thus if we choose the "scaling" of the weights so that R is the same in all six cases, then we have the same upper and lower bounds in each case, and thus the normalised worst-case errors would be roughly comparable.

How should we choose this number R? Clearly we have $R > 1$ and it follows from the upper bound that a small value of R means small normalised worst-case errors. On the other hand, if R is large compared to n, then it is possible for the lower bound to be greater than 1, which means that the worst-case error can be larger than the initial error. To ensure that this never happens, we take $R = 2$, which leads to a value of 1 for both the upper and lower bounds at $n = 1$.

Remark 4.3.2 By rescaling the weights, as above, we make them dependent on d; whereas so far we assumed that γ_j's are independent of d. The latter assumption was made only for the simplicity of presentation and the results of this paper can be easily generalized to the case of $\gamma_j = \gamma_{d,j}$ depending on d. The problem of finding a good scaling for the weights was already considered in [13] with a conclusion that *the sum of the weights* should be in a certain range (e.g., between d and $2d$) to reduce the error. Our approach here is very similar and, in particular, the quantity R corresponds to an exponential function of the sum of weights. For the purpose of our experiments here, we consider $d = 100$ to be given and fixed, and we treat the scaling factors in each case as if they were constants.

Our next step is to compute the price of the Asian call option using these newly constructed randomly-shifted lattice rules. Each evaluation of the integral I_d uses a random shift; we carry out 10 such evaluations $Q_1, \ldots, Q_{10}$ using 10 independent random shifts and we take the average $\overline{Q} = (Q_1 + \cdots + Q_{10})/10$ as our final approximation to the integral I_d. An unbiased estimate of the standard error for this approximation can be computed by

$$\sqrt{\frac{1}{10} \times \frac{1}{9} \sum_{i=1}^{10} (Q_i - \overline{Q})^2}.$$

The results are presented in Tables 4.1–4.3. Each table contains the estimated standard errors using those randomly-shifted lattice rules generated in the three cases based on a particular style and a specific scaling of weights. The scaling

factors are included in the third row of each table. For example, the weights for the case of a Gaussian ψ with $\alpha = 5$ in Table 4.1 are given by $\gamma_j \approx 0.773/j^2$. These seemingly arbitrary scaling factors were chosen to keep $R = 2$ within each table. The last row of each table corresponds to the observed order of convergence $\mathcal{O}(n^{-a})$, which is estimated by taking a least squares fit. Also included in the final column of Tables 4.1–4.3 are the standard errors in the Sobolev space *anchored* at the center of the unit cube $(1/2, \ldots, 1/2)$. Recall Section 2.4.3 and specifically (2.25) for a discussion of the anchored Sobolev space. As a comparison, Table 4.4 includes results obtained from three sets of calculations using Monte Carlo methods. All entries were computed using the same 10 random shifts. We report here only the results from the PCA construction since it consistently gives better QMC approximations than the standard construction. The PCA construction has the effect of reallocating most of the variance to the first few integration variables, thus reducing the *effective dimension* of the problem (see [1, 60]). Note that it has no effect on MC approximations, since the MC error depends only on the total variance of the integrand, which is unchanged under the PCA construction.

n	ψ Gaussian	ψ two-tailed	ψ logistic	Sobolev
	$\alpha = 5$	$\alpha = 2$	$\alpha = 2$	
	7.73e-01	3.71e-01	5.34e-02	3.35e+00
1009	6.23e-03	6.49e-03	6.97e-03	6.60e-03
2003	3.12e-03	3.03e-03	3.02e-03	2.87e-03
4001	1.32e-03	1.28e-03	1.32e-03	1.42e-03
8009	8.21e-04	7.90e-04	7.54e-04	8.54e-04
16001	4.68e-04	5.29e-04	5.33e-04	4.37e-04
32003	2.65e-04	3.01e-04	2.87e-04	2.62e-04
64007	9.55e-05	8.49e-05	8.59e-05	9.12e-05
a	0.95	0.96	0.97	0.97

Table 4.1: Standard errors for Asian option problem with $\gamma_j \propto 1/j^2$

n	ψ Gaussian	ψ two-tailed	ψ logistic	Sobolev
	$\alpha = 5$	$\alpha = 2$	$\alpha = 2$	
	1.15e-01	5.63e-02	7.87e-03	4.79e-01
1009	7.00e-03	5.98e-03	6.35e-03	6.17e-03
2003	2.87e-03	2.56e-03	3.10e-03	3.05e-03
4001	1.31e-03	1.27e-03	1.26e-03	1.24e-03
8009	7.33e-04	7.78e-04	7.74e-04	7.38e-04
16001	4.53e-04	5.48e-04	4.86e-04	4.89e-04
32003	2.69e-04	2.77e-04	2.63e-04	2.72e-04
64007	9.92e-05	9.56e-05	1.03e-04	9.01e-05
a	0.96	0.91	0.94	0.95

Table 4.2: Standard errors for Asian option problem with $\gamma_j \propto 0.9^j$

We see from the numbers that, regardless of the choice of ψ, the rules from our new spaces perform as well as the rules from the anchored Sobolev spaces. The empirical rate of convergence is *much better* than the theoretically predicted $\mathcal{O}(n^{-1/2})$, that is, $a = 0.5$. This suggests that it is possible to construct lattice rules which achieve the optimal rate of convergence. Whether this is true or not remains an open problem.

We must stress once again that the integrand from the Asian option problem lies in neither the anchored Sobolev spaces nor in our $\mathcal{H}_{\text{unb},d,\boldsymbol{\gamma}}$ spaces. It fails to lie in the Sobolev spaces for two reasons: it is unbounded at the boundaries of the unit cube and its mixed first derivatives do not exist. With the spaces $\mathcal{H}_{\text{unb},d,\boldsymbol{\gamma}}$, the first of these problems is remedied; however, the second is yet to be rectified.

4.4 Discussion

In this chapter we provide a CBC algorithm for constructing randomly-shifted lattice rules to approximate multivariate ρ_d-weighted integrals with the worst-

n	ψ Gaussian	ψ two-tailed	ψ logistic	Sobolev
	$\alpha = 5$	$\alpha = 2$	$\alpha = 2$	
	1.01e-02	4.96e-03	6.90e-04	4.19e-02
1009	7.11e-03	5.78e-03	6.61e-03	7.17e-03
2003	2.99e-03	3.14e-03	3.04e-03	2.81e-03
4001	1.29e-03	1.10e-03	1.39e-03	1.33e-03
8009	7.83e-04	6.65e-04	7.52e-04	7.86e-04
16001	4.67e-04	4.87e-04	5.10e-04	4.58e-04
32003	2.62e-04	2.60e-04	2.73e-04	2.77e-04
64007	9.53e-05	9.35e-05	9.42e-05	1.00e-04
a	0.97	0.94	0.96	0.95

Table 4.3: Standard errors for Asian option problem with $\gamma_j \propto 1$

case error at least proportional to $1/\sqrt{n}$. This result holds for a rather wide class of integrands: the function space can be tuned, by way of an additional weight function ψ, to suit a specific application. That is, for a given integrand, one can choose the weight ρ to write the integral in the form (4.1), and next the weight ψ. Once (4.3) and (4.4) are satisfied, and the corresponding norm of g exists, one can then apply the CBC algorithm.

We stress that for any specific application, there is no unique pair (ρ, ψ) satisfying (4.3) and (4.4). Unfortunately, choosing the *best* (or *almost best*) pair might be a difficult task. Nevertheless, we believe that this approach can be successfully used for many practical problems including numerous maximum likelihood integrals in statistics (see, e.g., [6]). It can also be used for integrands that cannot be modeled by any choice of (ρ, ψ) as illustrated by the numerical experiments with the Asian option problem.

n	MC 1	MC 2	MC 3
1009	9.63e-02	7.23e-02	8.98e-02
2003	8.25e-02	7.01e-02	6.54e-02
4001	3.56e-02	4.17e-02	2.82e-02
8009	3.33e-02	2.20e-02	3.35e-02
16001	1.73e-02	2.25e-02	1.79e-02
32003	1.45e-02	1.23e-02	1.25e-02
64007	1.01e-02	1.51e-02	1.45e-02
a	0.57	0.45	0.48

Table 4.4: Standard errors for Asian option problem with Monte Carlo methods

Chapter 5

Lattice rules extensible in the number of points

We have seen that an n-lattice rule with generating vector $\boldsymbol{z}$ and (random) shift $\boldsymbol{\Delta}$ gives us an n-point point set $P_{n,d}$ with points

$$\left\{\frac{k\boldsymbol{z}}{n}+\boldsymbol{\Delta}\right\}, \quad \text{for } k=0,1,\ldots,n \quad 1.$$

We see that each point in the lattice is explicitly dependent on the number of points n. This is not a desirable feature for a practitioner.

We saw in Section 2.4.5 that using a number of random shifts of given point set, we are able to make an unbiased estimate of the standard error of an approximation to the integration problem. A practitioner may wish to only use as many points as are necessary so the the standard error is within some bound. This is difficult with lattice rules as the value of n must be decided *before* the standard error can be calculated.

There are several QMC alternatives to lattice rules which do not have this problem. Point sets based on Sobol' points [58], Kronecker type sequences [38, 39, 42] and digital nets and sequences, see [41, 42, 44].

Though a desirable property [23], a generating vector which is good for many different values of n has until now not been constructed with either the Korobov or CBC-type algorithms.

5.1 Extensible lattice rules

The theoretical existence of generating vectors which have small worst-case error for a number of different values of n has been shown in [24]. The lattice rules generated from such vectors are nowadays called *extensible lattice rules*. In this case the quadrature points are given by $\boldsymbol{t}_k = \{\varphi(k)\boldsymbol{z} + \boldsymbol{\Delta}\}$, where $k = k_0 + k_1 p + \cdots + k_m p^m$ for $k = 0, 1, \ldots, n-1$ and the radical inverse function φ is defined by $\varphi(k) = k_0 p^{-1} + \cdots + k_m p^{-m-1}$. Here $\boldsymbol{z}$ is a vector of p-adic numbers. (See [26] for a definition of p-adic numbers; for our purposes here it is enough to assume that $\boldsymbol{z}$ is a vector of natural numbers hence we will not introduce p-adic numbers here.)

The existence of good extensible lattice rules has been proven in [26] (see Section 5.5 about a discussion of the precise meaning of "extensible"). Therein it was shown that there exists a generating vector $\boldsymbol{z}$ which yields a lattice rule which is good for $n = b, b^2, b^3, \ldots$, for any integer $b \geq 2$. The proof is based on a more sophisticated averaging argument. It should be noted that the lattice rules whose existence was proven in [26] are extensible in both the number of points *and* the dimension. They share this property with lattice rules constructed by the CBC algorithm. After the existence had been established it remained a challenge to provide some construction algorithm which yields generating vectors for extensible lattice rules. Several successful numerical investigations have been carried out [4, 25], but a proof that those algorithms yield good extensible lattice rules was not provided.

In this chapter we provide such an algorithm together with a proof. The argument for the proof is indeed similar to the one used in [26]. It uses a combination of Markov's inequality, Jensen's inequality and an extension of the following simple fact: let A, B be two subsets of a finite set N and let $|N|$ denote the number of elements in N. Then $|A|, |B| > |N|/2$ implies that $A \cap B \neq \emptyset$. (We use an extension of this to an arbitrary number of subsets of N.) Using these principles we can obtain both an algorithm and a proof, thereby

providing first construction algorithms for extensible lattice rules. To speed up the algorithm we show that we can also use a CBC approach (as described in Section 2.6.2) together with the fast CBC computation method (as described in Section 2.6.3). This way we obtain a practically feasible construction of extensible lattice rules in (for many applications) sufficiently large dimensions and a range of values of n.

Unfortunately our construction algorithms are not extensible in both n and d simultaneously. The first sieve algorithm (see Section 5.2), though slow, is in principle extensible in n, but is not extensible in the dimension. The CBC sieve algorithm and the fast CBC sieve algorithm (see Section 5.3) construct generating vectors for a range of moduli and is extensible in the dimension, but once the vector is constructed it is not possible to extend the vector to work well also for other moduli. Hence the CBC sieve constructions provide embedded rather then extensible lattice rules [4]. Obtaining an algorithm which is extensible in both n and d simultaneously remains an interesting open question. See also Section 5.5 at the end of the chapter for a discussion of this topic.

The existence of good extensible lattice rules was originally proven by showing that the quantity R_α is small. (See [42] for a description of R_α.) It is possible to use our approach to minimise a similar quantity R (see [11] for details).

5.2 The sieve algorithm

In [26] the authors used p-adic numbers to show the existence of good extensible lattices. Basically we could use p-adic numbers too, but we focus on the construction of finitely extensible lattices by computer search. In theory, the lattice could be infinitely extensible if the computer were able to search for an infinite length of time. It is enough in our case to assume that the generating vector is in the set $\mathbb{N}^d$.

The paper [26] proved that it was possible to construct generating vectors $\boldsymbol{z}$ with small worst-case error for $n = b, b^2, b^3, \ldots$ for all integers $b \geq 2$. In this chapter, we will again consider p to be an arbitrary prime, rather than any integer, and we will show that lattice rules may be constructed for $n = p, p^2, p^3, \ldots$. However, it is almost trivial to extend the following construction algorithm to the case where $n = b, b^2, b^3, \ldots$ for all integers $b \geq 2$. See the Remarks 5.2.8 and 5.3.6.

Then we restrict the set of admissible generating vectors to $\mathcal{Z}_p^d$ as defined in (2.33). Clearly, there is an infinite number of elements in this set. Since $e_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\widehat{\boldsymbol{z}}) = e_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\overline{\boldsymbol{z}})$ if $\overline{\boldsymbol{z}} \equiv \widehat{\boldsymbol{z}} \pmod{p^m}$, we exploit the structure inherent in lattice rules by restricting our searches to the set $\mathcal{Z}_{p,m}^d$ as defined in (2.34). We will say that for $\overline{\boldsymbol{z}} \in \mathcal{Z}_p^d$, the vector $\widehat{\boldsymbol{z}}$ is the *corresponding* vector in $\mathcal{Z}_{p,m}^d$.

5.2.1 Bounds on the worst-case error

In this section we prove some essential results which will shed light on how we intend to construct good extensible lattice rules. Recall from Theorems 2.5.3 and 2.5.10 that for p such that $p \geq \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ and m and d positive integers there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_{p,m}^d$ such that

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}, \tag{5.1}$$

and more generally for all $\lambda \in (1/\alpha, 1]$

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda). \tag{5.2}$$

We wish to define a probability measure over the set of all generating vectors $\mathcal{Z}_p^d$ [26, 43]. We would like to do so such that the measure of corresponding vectors in $\mathcal{Z}_{p,m}^d$ is equiprobable. For $m \in \mathbb{N}$ let $\mu_{d,m}$ be the equiprobable measure on the set $\mathcal{Z}_{p,m}^d$. We say a subset A of $\mathcal{Z}_p^d$ is of finite type, if there exists an integer $m = m(A) \in \mathbb{N}$ and a subset A' of $\mathcal{Z}_{p,m}^d$ such that

$$A = \{\boldsymbol{z} \in \mathcal{Z}_p^d : (\boldsymbol{z} \pmod{p^m}) \in A'\}.$$

The measure of the finite type subset A is then defined as

$$\mu_d(A) = \mu_{d,m(A)}(A').$$

Thus,

$$\mu_d(A) = \frac{\#A'}{\phi(p^m)^d}. \tag{5.3}$$

(Of course the number $m = m(A)$ is not uniquely defined by A since if m works, then also any number larger than m will work in the definition of a finite type subset. It is easy to see that (5.3) does not depend on the specific choice of m.)

We now define the following set. For a real $c \geq 1$ let

$$\mathcal{C}_{n,d,\alpha,\boldsymbol{\gamma}}(c) = \{\boldsymbol{z} \in \mathcal{Z}_p^d \,:\, e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq cM^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}\}. \tag{5.4}$$

This set has the following property.

Theorem 5.2.1 *Let p be prime such that $p \geq \left(\frac{\gamma_1\zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ and let m and d be positive integers. For any $c \geq 1$ we have*

$$\mu_d(\mathcal{C}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c)) > 1 - c^{-1}.$$

Proof. This follows immediately from applying Markov's inequality to (5.1). □

We now make a small adjustment to this set which allows us to incorporate Jensen's inequality, see [13] where a similar argument was used. For a real $c \geq 1$ define the set

$$\widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c) = \{\boldsymbol{z} \in \mathcal{Z}_p^d \,:\, e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq c^{1/\lambda} M^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) \text{ for all } \lambda \in (1/\alpha, 1]\}. \tag{5.5}$$

We obtain the following theorem.

Theorem 5.2.2 *Let p be prime such that $p \geq \left(\frac{\gamma_1\zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$ and m and d be positive integers. For any $c \geq 1$ we have*

$$\mu_d(\widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c)) > 1 - c^{-1}.$$

Proof. Let $c \geq 1$ be given and choose $1/\alpha < \lambda^* \leq 1$ such that

$$c^{1/\lambda^*} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda^*) \leq c^{1/\lambda} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$, noting that the minimum can not occur at $\lambda^* = 1/\alpha$ since $M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(1/\alpha)$ is infinite. From Theorem 5.2.1 we see that

$$\mu_d(\mathcal{C}_{p^m,d,\alpha\lambda^*,\boldsymbol{\gamma}^{\lambda^*}}(c)) > 1 - c^{-1}. \tag{5.6}$$

Now, if $\boldsymbol{z} \in \mathcal{C}_{p^m,d,\alpha\lambda^*,\boldsymbol{\gamma}^{\lambda^*}}(c)$, then

$$e^2_{\mathrm{per},p^m,d,\alpha\lambda^*,\boldsymbol{\gamma}^{\lambda^*}}(\boldsymbol{z}) \leq c M^2_{\mathrm{per},p^m,d,\alpha\lambda^*,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^{\lambda^*}}.$$

By (2.42) this implies that

$$\left(e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})\right)^{\lambda^*} \leq c M^2_{\mathrm{per},p^m,d,\alpha\lambda^*,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^{\lambda^*}},$$

which can be re-written as

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq c^{1/\lambda^*} \left(M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}\right)^{1/\lambda^*} = c^{1/\lambda^*} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda^*),$$

which in turn implies that $\boldsymbol{z} \in \widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c)$. This means that $\mathcal{C}_{p^m,d,\alpha\lambda^*,\boldsymbol{\gamma}^{\lambda^*}}(c) \subseteq \widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c)$. Using (5.6) as a lower bound, we find that

$$\mu_d(\widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c)) \geq \mu_d(\mathcal{C}_{p^m,d,\alpha\lambda^*,\boldsymbol{\gamma}^{\lambda^*}}(c)) > 1 - c^{-1}.$$

□

In the following we will use the above theorem to construct lattices for a range of moduli.

5.2.2 The sieve principle

We now want to construct lattice rules which work well for several choices of m. Let p^{m_1} be the lowest number of points and p^{m_2} be the highest number of points in which we are interested in, i.e., $m_1 \leq m_2$. Then for each $m = m_1, m_1 + 1, \ldots, m_2$ we can define a set $\widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)$ as in (5.5). In order to

obtain a generating vector which works well for all choices of $m = m_1, \ldots, m_2$ we need to show that the intersection $\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)$ is not empty, or equivalently, has measure greater than 0. To this end choose $c_m \geq 1$ such that

$$\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1, \tag{5.7}$$

then the measure of the intersection of the sets above can be shown to be strictly positive.

In the following we will write $\widetilde{\mathcal{C}}^c_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)$ to denote the complement of the set $\widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)$ in $\mathcal{Z}_p^d$.

Theorem 5.2.3 *Let p be prime such that $p \geq \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$, d be a positive integer and let $0 < m_1 \leq m_2$. Let $c_m \geq 1$ for all $m = m_1, \ldots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$. Then there exists a vector $\boldsymbol{z} \in \mathcal{Z}_p^d$ such that*

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq c_m^{1/\lambda} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$ and $m = m_1, \ldots, m_2$.

Proof. We need to show that $\mu_d\left(\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)\right) > 0$. This is a simple calculation,

$$\begin{aligned}
\mu_d\left(\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)\right) &= 1 - \mu_d\left(\bigcup_{m=m_1}^{m_2} \widetilde{\mathcal{C}}^c_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)\right) \\
&\geq 1 - \sum_{m=m_1}^{m_2} \mu_d(\widetilde{\mathcal{C}}^c_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)) \\
&> 1 - \sum_{m=m_1}^{m_2} c_m^{-1} \;\geq\; 0.
\end{aligned}$$

□

The arguments used to prove Theorem 5.2.3 are very similar to the arguments used in [26]. (Using p-adic numbers we could indeed also allow m_2 to be infinite. As in [26], using the above arguments, it is also possible to show the existence of a large number of good generating vectors.) In the following section, we will demonstrate how this theory can also be used to construct good generating vectors.

5.2.3 The sieve algorithm

In this section we introduce the idea of how a good generating vector can be found by describing a sieve algorithm for the construction of a generating vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ which works well for $m = m_1, \ldots, m_2$. This algorithm is quite slow, but in later sections we will give some modifications which speed up the sieve algorithm.

We wish to find a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ which for $m = m_1, \ldots, m_2$ satisfies

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le c_m^{1/\lambda} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda), \quad \text{for all } \lambda \in (1/\alpha, 1].$$

That is, we wish to find a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ that lies in $\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d,\alpha,\boldsymbol{\gamma}}(c_m)$. For $m = m_1$ we use a computer search to find $\lfloor (1 - c_{m_1}^{-1})\phi(p^{m_1})^d \rfloor + 1$ of the $\phi(p^{m_1})^d$ vectors in $\mathcal{Z}_{p,m_1}^d$, which satisfy $e^2_{\mathrm{per},p^{m_1},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le c_{m_1}^{1/\lambda} M^2_{\mathrm{per},p^{m_1},d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $\lambda \in (1/\alpha, 1]$ and label this set T_{m_1}. By Theorem 5.2.2 we know that at least such a number of vectors exist.

We then construct the set S_{m_1+1} of all vectors $\boldsymbol{z} \in \mathcal{Z}_{p,m_1+1}^d$, such that there exists some $\overline{\boldsymbol{z}} \in T_{m_1}$ with $\boldsymbol{z} \equiv \overline{\boldsymbol{z}} \pmod{p^{m_1}}$. From the set S_{m_1+1} we only keep $\lfloor (1 - (c_{m_1}^{-1} + c_{m_1+1}^{-1}))\phi(p^{m_1+1})^d \rfloor + 1$ vectors which satisfy the inequality $e^2_{\mathrm{per},p^{m_1+1},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \le c_{m_1+1}^{1/\lambda} M^2_{\mathrm{per},p^{m_1+1},d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $\lambda \in (1/\alpha, 1]$ and label this set T_{m_1+1}. Again by Theorem 5.2.2 we know there must be at least

$$\lfloor (1 - c_{m_1+1}^{-1})\phi(p^{m_1+1})^d \rfloor + 1$$

vectors in $\mathcal{Z}_{p,m_1+1}^d$ which satisfy $e^2_{\mathrm{per},p^{m_1+1},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le c_{m_1+1}^{1/\lambda} M^2_{\mathrm{per},p^{m_1+1},d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $\lambda \in (1/\alpha, 1]$. Therefore, there must be at least

$$\lfloor (1 - (c_{m_1}^{-1} + c_{m_1+1}^{-1}))\phi(p^{m_1+1})^d \rfloor + 1$$

vectors which satisfy $e^2_{\mathrm{per},p^{m_1},d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le c_{m_1}^{1/\lambda} M^2_{\mathrm{per},p^{m_1},d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $\lambda \in (1/\alpha, 1]$ as well.

In the same way, we construct the sets $S_{m_1+2}, T_{m_1+2}, \ldots, S_{m_2}$ and T_{m_2}. By Theorem 5.2.3 above, T_{m_2} is guaranteed not to be empty. We may select $\boldsymbol{z}^*$ to be any vector from T_{m_2} (see Section 5.3.2 for some comments on how to choose a vector from T_{m_2}).

Remark 5.2.4 In principle we can allow m_2 to be infinite, i.e., we can choose c_m such that $\sum_{m=m_1}^{\infty} c_m^{-1} \leq 1$. Then we can stop the computer search at some finite $m' > m_1$. If one stores all the necessary values from the initial search it is then also possible to resume the computer search at a later point in time to obtain an extensible lattice rules also for moduli larger than $p^{m'}$. Hence the construction is truly extensible in the modulus (see also Section 5.5 for more information on extensibility). As we will show in the next section, the vector can also be extended in the dimension using a CBC approach, but once this is done, it becomes "embedded" (see [4]) rather than extensible in the modulus, since the values of m_1 and m_2 may not be altered once chosen.

Further, as can be seen from the arguments above, one need not choose successive values of m, i.e., one could choose an arbitrary subset $K \subset \mathbb{N}$ and construct a good lattice rule with p^m points for all $m \in K$.

Remark 5.2.5 The constants $c_m \geq 1$ for $m = m_1, \ldots, m_2$ may be chosen to be any positive sequence of reals such that (5.7) is satisfied. If m_2 is finite, one possible choice of c_m to satisfy (5.7) is $c_m = m_2 - m_1 + 1$. This corresponds to the lattice rule having in some sense the same quality for each value of m. This choice will be used later in Section 5.4.

If m_2 is chosen to be infinite, we cannot choose c_m to be independent of m as we did above. Instead, the constants c_m must grow with m sufficiently fast so that the sum in (5.7) converges. One possible choice is $c_m = Cm(\log(m+1))^{1+\epsilon}$ for any $\epsilon > 0$ where C is chosen to be larger than $\sum_{m=m_1}^{\infty} m^{-1}(\log(m+1))^{-(1+\epsilon)}$. This is the choice used in [26]. A similar choice would be $c_m = \zeta(1+\epsilon)m^{1+\epsilon}$ again for any $\epsilon > 0$.

The following theorem now applies to generating vectors constructed by the sieve algorithm.

Theorem 5.2.6 *Let p be prime such that $p \geq \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$, d be a positive integer and let $0 < m_1 \leq m_2$. Let $c_m \geq 1$ for all $m = m_1, \ldots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$. Then the sieve algorithm constructs a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ such*

that

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le c_m^{1/\lambda} M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$ *and* $m = m_1, \ldots, m_2$.

Note that it is always possible to choose c_m of order $m^{1+\varepsilon}$ for any $\varepsilon > 0$, hence the factor c_m in the bound in the above theorem contributes at most another factor of $m^{(1+\varepsilon)/\lambda} = (\log n)^{(1+\varepsilon)/\lambda}$, where n is the number of points. It can be shown that for every $0 < \delta < 1$ there is a constant $D_\delta > 0$ such that $(\log n)^c n^{-1} \le D_\delta n^{-\delta}$, hence for every $\lambda \in (1/\alpha, 1]$ there is a constant $C_\lambda > 0$ such that

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le C_\lambda p^{m/\lambda} \prod_{j=1}^{d} \left(1 + 2\gamma_j^\lambda \zeta(\alpha\lambda)\right)^{1/\lambda}$$

for all $m = m_1, \ldots, m_2$. (Here the constant C_λ may depend on the particular choice of c_m; on the other hand there is also a constant C_λ even if $m_2 = \infty$, see [26]). So using the sieve algorithm we can construct generating vectors for lattice rules which achieve the optimal rate of convergence for a range of moduli.

Remark 5.2.7 In the theorems above, we have always made the assumption that p is chosen such that $p \ge \left(\frac{\gamma_1 \zeta(\alpha)}{2\pi^2}\right)^{1/\alpha}$. If we replace $M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ with $\overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ in each theorem, we can see that we can drop the condition on p.

Remark 5.2.8 Following Remark 2.5.9, we see that the above theorems also hold if $M^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ is replaced by $\widetilde{M}^2_{\mathrm{per},b^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for an arbitrary positive integer $b \ge 2$.

5.3 CBC construction

In the previous section we gave the idea of how to construct extensible lattice rules. In this section we show that the sieve algorithm can be combined with a CBC approach (as discussed in Section 2.6.2) to obtain a faster construction

algorithm which will allow us to construct good lattice rules for a practically relevant range of moduli and dimensions. This also gives the added benefit of obtaining a construction which is also extensible in the dimension, but unfortunately the range of moduli in this case has to be chosen in advance and cannot be extended anymore. In this sense our lattice rules are embedded rather then extensible, see also Section 5.5 and [26].

5.3.1 The CBC sieve algorithm

We may reduce the construction cost by constructing the vector $\boldsymbol{z}^*$ component-by-component. This approach has been shown to be very useful and effective in constructing lattice rules for fixed n where one has $\phi(n)^d$ choices of $\boldsymbol{z}$. Recall that the CBC algorithm works the following way: choose the first component of the generating vector $z_1^* = 1$. Then, for $\boldsymbol{z}_d^* = (z_1^*, \ldots, z_d^*)$ already chosen, we will choose a component z_{d+1}^* such that the worst-case error $e_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*)$ satisfies a certain bound. This way we can obtain a good generating vector inductively.

We will now establish a similar sequence of theorems to those of Theorems 5.2.1–5.2.3 which now include the component-by-component approach. Since we construct a vector $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1})$ with $\boldsymbol{z}_d^*$ fixed, we are concerned only with the incremental impact of the choice of z_{d+1} on the worst-case error.

Recall the definition from (2.45)

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) = e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1})) - e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*),$$

and the fact that

$$\frac{1}{\phi(p^m)} \sum_{z_{d+1} \in \mathcal{Z}_{p,m}} \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \le \overline{\theta}_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}} \tag{5.8}$$

where

$$\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}} = \frac{4}{p^m} \frac{\gamma_{d+1}}{2\pi^2} \zeta(\alpha) \prod_{j=1}^{d} \left(1 + 2\frac{\gamma_j}{2\pi^2}\zeta(\alpha)\right).$$

We now define a set which is analogous to (5.4). For a real $c \geq 1$ and $\boldsymbol{z}_d^* \in \mathcal{Z}_p^d$ let

$$\mathcal{C}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c;\boldsymbol{z}_d^*) = \{z_{d+1} \in \mathcal{Z}_p \,:\, \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \leq c\,\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}\}. \tag{5.9}$$

The following theorem follows immediately from Markov's inequality. Recall that each term $\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$ is non-negative as seen in (2.48) and hence Markov's inequality can be applied. As in this section we only deal with sets of one-dimensional vectors we simply write μ for the measure μ_1.

Theorem 5.3.1 *Let m and d be positive integers and p prime. Then for any $c \geq 1$ we have*

$$\mu(\mathcal{C}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c\,;\boldsymbol{z}_d^*)) > 1 - c^{-1}.$$

Proof. This follows immediately from applying Markov's inequality to (5.8). □

We will be able to achieve stronger convergence results for the worst-case error if we use Jensen's inequality. We define the set

$$\begin{aligned}\widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c;\boldsymbol{z}_d^*) = \Big\{ & z_{d+1} \in \mathcal{Z}_p \,:\, \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \\ & \leq c^{1/\lambda} \left(\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}\right)^{1/\lambda} \text{ for all } \lambda \in (1/\alpha, 1]\Big\}.\end{aligned} \tag{5.10}$$

This new set has the following property.

Theorem 5.3.2 *Let m and d be positive integers and p prime. Then for any $c \geq 1$ we have*

$$\mu(\widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c;\boldsymbol{z}_d^*)) > 1 - c^{-1}.$$

Proof. From Theorem 5.3.1 we can say

$$\mu(\widetilde{\mathcal{C}}_{p^m,d+1,\alpha\lambda,\boldsymbol{\gamma}^\lambda}(c;\boldsymbol{z}_d^*)) > 1 - c^{-1}. \tag{5.11}$$

Now, if $z_{d+1} \in \mathcal{C}_{p^m,d+1,\alpha\lambda,\boldsymbol{\gamma}^\lambda}(c;\boldsymbol{z}_d^*)$ then

$$\theta_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}(\boldsymbol{z}_d^*, z_{d+1}) \leq c\,\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\boldsymbol{\gamma}}{2\pi^2})^\lambda}.$$

Applying Jensen's inequality to (2.48) we see that

$$(\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}))^\lambda \leq \theta_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}(\boldsymbol{z}_d^*, z_{d+1}).$$

Combining the last two inequalities implies

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \leq c^{1/\lambda} \left(\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}\right)^{1/\lambda}$$

which implies that $z_{d+1} \in \widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c; \boldsymbol{z}_d^*)$. It then follows immediately that $\mathcal{C}_{p^m,d+1,\alpha\lambda,\boldsymbol{\gamma}^\lambda}(c; \boldsymbol{z}_d^*) \subseteq \widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c; \boldsymbol{z}_d^*)$, which by using (5.11) as a lower bound implies that

$$\mu(\widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c; \boldsymbol{z}_d^*)) \geq \mu(\mathcal{C}_{p^m,d+1,\alpha\lambda,\boldsymbol{\gamma}^\lambda}(c; \boldsymbol{z}_d^*)) > 1 - c^{-1}.$$

□

In the same vein as Theorem 5.2.3, we show in the following theorem that there exists a component $z_{d+1}^* \in \mathcal{Z}_p$ such that the squared worst-case error $e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*)$ is small for all $m = m_1, \ldots, m_2$.

Theorem 5.3.3 *Let m and d be positive integers and p prime. Let $\boldsymbol{z}_d^* \in \mathcal{Z}_p^d$. Let $c_m \geq 1$ for all $m = m_1, \ldots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$. Then there exists a $z_{d+1}^* \in \mathcal{Z}_p$ such that*

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \leq c_m^{1/\lambda} \left(\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}\right)^{1/\lambda}$$

for all $\lambda \in (1/\alpha, 1]$ and $m = m_1, \ldots, m_2$.

Proof. We need to show that $\mu\left(\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c_m; \boldsymbol{z}_d^*)\right) > 0$. This is a simple calculation,

$$\begin{aligned}
\mu\left(\bigcap_{m=m_1}^{m_2} \widetilde{\mathcal{C}}_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c_m; \boldsymbol{z}_d^*)\right) &= 1 - \mu\left(\bigcup_{m=m_1}^{m_2} \widetilde{\mathcal{C}}^c_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c_m; \boldsymbol{z}_d^*)\right) \\
&\geq 1 - \sum_{m=m_1}^{m_2} \mu(\widetilde{\mathcal{C}}^c_{p^m,d+1,\alpha,\boldsymbol{\gamma}}(c_m; \boldsymbol{z}_d^*)) \\
&> 1 - \sum_{m=m_1}^{m_2} c_m^{-1} \;\geq\; 0.
\end{aligned}$$

□

We can put the existing vector $\boldsymbol{z}_d^*$ together with the new component z_{d+1}^* to show that the vector $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$ has the following properties.

Theorem 5.3.4 *Let m and d be positive integers and p prime. Let $\boldsymbol{z}_d^*$ be chosen so that*

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \le c_m^{1/\lambda}\, \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

and z_{d+1}^* be chosen so that

$$\theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \le c_m^{1/\lambda} \left(\overline{\theta}_{\mathrm{per},p^m,d+1,\alpha\lambda,2\pi^2(\frac{\gamma}{2\pi^2})^\lambda}\right)^{1/\lambda}$$

for all $\lambda \in (1/\alpha, 1]$. Then

$$e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d+1}^*) \le c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$, where $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$.

Proof. We have

$$\begin{aligned}
&e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) = e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) + \theta_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}^*) \\
&\le \frac{c_m^{1/\lambda}}{p^{m/\lambda}} \left(\prod_{j=1}^{d} \left(1 + 4\gamma_j^\lambda \zeta(\alpha\lambda)\right) - 1\right)^{1/\lambda} \\
&+ \frac{c_m^{1/\lambda}}{p^{m/\lambda}} \left(4\gamma_{d+1}^\lambda \zeta(\alpha\lambda) \prod_{j=1}^{d} \left(1 + 4\gamma_j^\lambda \zeta(\alpha\lambda)\right)\right)^{1/\lambda} \\
&\le \frac{c_m^{1/\lambda}}{p^{m/\lambda}} \left(\prod_{j=1}^{d} \left(1 + 4\gamma_j^\lambda \zeta(\alpha\lambda)\right) - 1 + 4\gamma_{d+1}^\lambda \zeta(\alpha\lambda) \prod_{j=1}^{d} \left(1 + 4\gamma_j^\lambda \zeta(\alpha\lambda)\right)\right)^{1/\lambda} \\
&= \frac{c_m^{1/\lambda}}{p^{m/\lambda}} \left(\prod_{j=1}^{d+1} \left(1 + 4\gamma_j^\lambda \zeta(\alpha\lambda)\right) - 1\right)^{1/\lambda} = c_m^{1/\lambda}\, \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda),
\end{aligned}$$

where the second inequality uses another application of Jensen's inequality. □

We may now construct the extensible generating vector $\boldsymbol{z}^*$ using the CBC method. The algorithm to do this is stated formally in Algorithm 4.

Algorithm 4 CBC construction of $\boldsymbol{z}^*$ with small $e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$ for $m = m_1, \ldots, m_2$

Require: $m_1 \le m_2 \in \mathbb{N}_0$, $\alpha > 1$, a positive sequence of weights $\boldsymbol{\gamma}$, p and $d_{\max}$ positive integers and a sequence $c_{m_1}, \ldots, c_{m_2}$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \le 1$

Set $z_1^* = 1$

for $s = 1$ to $d_{\max} - 1$ **do**

Find $\lfloor (1 - c_{m_1}^{-1})\phi(p^{m_1}) \rfloor + 1$ components $z_{d+1} \in \mathcal{Z}_{p,m_1}^d$ to populate the set

$$T_{m_1,d+1} \subseteq \{z_{d+1} \in \mathcal{Z}_{p,m_1}^d \, : \, e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \le c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda) \text{ for all } \lambda \in (1/\alpha, 1]\}.$$

for $m = m_1 + 1$ to m_2 **do**

Define the set

$$S_{m,d+1} = \{z_{d+1} \in \mathcal{Z}_{p,m} \, : \, \exists \, \overline{z} \in T_{m-1,d+1} \text{ such that } z_{d+1} \equiv \overline{z} \pmod{p^{m-1}}\}$$

Find $\lfloor (1 - \sum_{i=m_1}^{m} c_i^{-1})\phi(p^m) \rfloor + 1$ vectors to populate the set

$$T_{m,d+1} \subseteq \{z_{d+1} \in S_{m,d+1} \, : \, e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \le c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda) \text{ for all } \lambda \in (1/\alpha, 1]\}.$$

end for

Select $z_{d+1}^* \in T_{m_2,d+1}$

Set $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$

end for

Set $\boldsymbol{z}^* = \boldsymbol{z}_{d_{\max}}^*$

Theorem 5.3.5 *Let d be a positive integer and $0 < m_1 \le m_2$. Let $c_m \ge 1$ for all $m = m_1, \dots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \le 1$. Then Algorithm 4 constructs a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ such that*

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \le c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$ and $m = m_1, \dots, m_2$.

Remark 5.3.6 Again we may generalise this result to n being the power of an arbitrary integer $b \ge 2$ by replacing $\overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ with $\widetilde{M}^2_{\mathrm{per},b^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$.

5.3.2 Optimising the CBC sieve algorithm

The classical CBC algorithm constructs one component of the generating vector at a time. For each dimension, it takes the component which minimises the worst-case error. The requirement that this component is the minimum is important in using Jensen's inequality to gain the optimal rate of convergence (see [35]). The sieve algorithm does not have this requirement. Rather than finding the minimiser at each step, we require a certain number of admissible vectors, that is, vectors whose worst-case error is lower than some bound. Therefore, Algorithm 4 will find an extensible lattice rule without the need for any optimisation.

However, it is instinctive that we should attempt to go beyond looking for simply a set of admissible vectors and attempt to find the *best* (in some sense) generating vectors at each step. This can be done by modifying the choice of the set $T_{m,d+1}$ for $m = m_1, \dots, m_2$ and $d = 1, \dots, d_{\max} - 1$ in Algorithm 4. Rather than just constructing $T_{m,d+1}$ with the first $\lfloor (1 - \sum_{i=m_1}^{m} c_i^{-1}) \phi(p^m) \rfloor + 1$ components z_{d+1} such that

$$e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1}) \le c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$, we construct the set $T_{m,d+1}$ to contain *all* components that satisfy the bound. We then truncate the set $T_{m,d+1}$ to contain exactly

those $\lfloor (1-\sum_{i=m_1}^{m} c_i^{-1})\phi(p^m) \rfloor + 1$ elements which have the smallest worst-case error $e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*, z_{d+1})$, for the given $\boldsymbol{z}_d^*$. As we will see in the numerical section, the bound is significantly larger than the actual errors and hence using such an optimisation step ensures that we do not choose any component which merely satisfies the bound but rather one that is amongst the best possibilities.

5.3.3 The fast CBC sieve algorithm

In the previous section we constructed the components of the generating vector by first choosing the first m_1 digits and then extending those up to m_2 digits step-by-step for a set of good components. Though this algorithm is feasible for practical values, it does not allow us to use the fast CBC algorithm introduced by Nuyens and Cools mentioned in Section 2.6.3. Their construction algorithm reduces the usual construction cost of the CBC algorithm from $O(dn^2)$ to $O(dn \log n)$ (which is a remarkable speed-up for large n) by exploiting the structure of the calculation.

In order to make use of the fast CBC algorithm we modify the previous construction algorithms. In this case it is necessary to search over all possible choices of the new component z_{d+1}, rather than just those which have been shown to be *good* for earlier values of m. Here we simply store all the *good* components z_{d+1} for the generating vector $(\boldsymbol{z}_d^*, z_{d+1})$ for each value of m. The construction is then performed by minimising a new error measure, which, for given $\boldsymbol{z}_d^* \in \mathcal{Z}_{p,m_2}^d$, is defined by

$$F_{m_1,m_2,d+1,\alpha,\boldsymbol{\gamma}}(z_{d+1}) = \sum_{m=m_1}^{m_2} \max_{\lambda \in (1/\alpha,1]} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))}{c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda)}. \tag{5.12}$$

Using this measure we now construct a generating vector one component at a time, in each step choosing z_{s+1}^* which minimises the quantity $F_{m_1,m_2,d+1,\alpha,\boldsymbol{\gamma}}$.

We can now use Theorem 5.3.3 to show that there must be at least one choice of $z_{d+1} \in \mathcal{Z}_p$ which is good for all $m = m_1, \ldots, m_2$.

Algorithm 5 Fast CBC sieve construction of a good generating vector $\boldsymbol{z}^*$ with small $e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$

Require: $m_1 \le m_2 \in \mathbb{N}_0$, $\alpha > 1$, a positive sequence of weights $\boldsymbol{\gamma}$ and $d_{\max}$ positive integers and the positive sequence $c_{m_1}, \dots, c_{m_2}$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \le 1$

1: Set $z_1^* = 1$

2: **for** $d = 1$ to $d_{\max} - 1$ **do**

3: **for** $m = m_1$ to m_2 **do**

4: Compute $\lambda_m^* \in (1/\alpha, 1]$ which minimises

$$N_{m,c_m}(\lambda) = c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda)$$

as a function of λ.

5: For each $z_{d+1,m} \in \mathcal{Z}_{p,m}$ compute

$$\frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))}{N_{m,c_m}(\lambda_m^*)}.$$

6: **end for**

7: Set

$$T_{d+1} = \left\{ z_{d+1} \in \mathcal{Z}_{p,m_2} : \max_{m_1 \le m \le m_2} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))}{N_{m,c_m}(\lambda_m^*)} \le 1 \right\}.$$

8: Select $z_{d+1}^* \in T_{d+1}$ which minimises

$$\sum_{m=m_1}^{m_2} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))}{N_{m,c_m}(\lambda_m^*)}$$

.

9: Set $\boldsymbol{z}_{d+1}^* = (\boldsymbol{z}_d^*, z_{d+1}^*)$

10: **end for**

11: Set $\boldsymbol{z}^* = \boldsymbol{z}_{d_{\max}}^*$

Theorem 5.3.7 *Let d be a positive integer, p prime and $0 < m_1 \leq m_2$. Let $c_m \geq 1$ for all $m = m_1, \ldots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$. Then Algorithm 5 constructs a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ such that*

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \leq c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$ and $m = m_1, \ldots, m_2$.

Remark 5.3.8 In Algorithm 5 note that instead of choosing $z^*_{d+1} \in T_{d+1}$ which minimises the quantity

$$\sum_{m=m_1}^{m_2} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}^*_d, z_{d+1}))}{N_{m,c_m}(\lambda^*_m)}$$

it would be enough in theory to pick any $z^*_{d+1} \in T_{d+1}$ (which must be non-empty by Theorems 5.3.3 and 5.3.4). But as searching for the minimum increases the construction cost only marginally it is advisable to include this step since the bound is typically very loose (see Section 5.4). Note that another legitimate choice in line 8 would be to select the $z^*_{d+1} \in T_{d+1}$ which minimises

$$F'_{m_1,m_2,d+1,\alpha,\gamma}(z_{d+1}) = \max_{m_1 \leq m \leq m_2} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}^*_d, z_{d+1}))}{N_{m,c_m}(\lambda^*_m)}. \tag{5.13}$$

In this instance we have chosen the former because it gives smaller worst case errors in the numerical experiments.

The minimum of $N_{m,c_m}(\lambda)$ can be found with sufficient accuracy using any standard one-dimensional constrained optimisation software. Computing the normalised worst-case error Algorithm 5 can be done in order $n \log n$ operations using the fast CBC algorithm.

5.3.4 Theoretical bounds on the algorithm of Cools et al

Algorithm 5 is very similar in nature to the algorithm suggested in [4]. Their algorithm is different in that given $\boldsymbol{z}^*_d$ they choose z^*_{d+1} to minimise the error

measure defined by

$$V_{p,m_1,m_2,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1})) = \max_{m_1 \le m \le m_2} \frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))}{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)})} \tag{5.14}$$

for $d = 1, \ldots, d_{\max} - 1$ where $\boldsymbol{z}^{(m)}$ is the generating vector with the CBC algorithm for $n = p^m$ for $m = m_1, \ldots, m_2$. In [4] there was no formal proof with any bound on the size of the error measure $V_{p,m_1,m_2,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$, although the numerical experiments suggested that it remained small.

Observe that the quality measures $F'_{m_1,m_2,d+1,\alpha,\gamma}(z_{d+1})$, which is given by (5.13), and $V_{p,m_1,m_2,d+1,\alpha,\boldsymbol{\gamma}}((\boldsymbol{z}_d^*, z_{d+1}))$ used in [4] are very similar. Indeed we will show in the following that with a few slight modifications we can change Algorithm 5 such that it is the same as the algorithm considered in [4].

Let $\lambda'_{m_1}, \ldots, \lambda'_{m_2} \in (1/\alpha, 1]$ (we will see later how those values could be chosen) and let

$$c_m = \left(\frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)})}{\overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_m)} \right)^{\lambda'_m} \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^(,d+1,\alpha,\boldsymbol{\gamma}}\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{\lambda'_m \alpha}. \tag{5.15}$$

Further choose λ^*_m in Algorithm 5 as λ'_m and select z^*_{d+1} in line 8 by minimising $F'_{m_1,m_2,d+1,\alpha,\gamma}(z_{d+1})$ with the constant c_m given by (5.15). Then

$$N_{m,c_m}(\lambda'_m) = c_m^{1/\lambda'_m} \overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_m) = C e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)}),$$

where

$$C = \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{\alpha}$$

is independent of m. This way we obtain the same algorithm as proposed by [4]. Note that the constant C does not have any influence on which z^*_{d+1} will be chosen and can actually be left out in Algorithm 5.

The basic principles used to obtain Theorem 5.3.7 now still apply as long

as $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$, that is

$$\begin{aligned}
&\sum_{m=m_1}^{m_2} c_m^{-1} \\
&= \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{-\lambda'_m \alpha} \sum_{m=m_1}^{m_2} \left(\frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)})}{\overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_m)} \right)^{-\lambda'_m} \\
&\leq \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{-1} \sum_{m=m_1}^{m_2} \left(\frac{e^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)})}{\overline{M}^2_{\mathrm{per},p^m,d+1,\alpha,\boldsymbol{\gamma}}(\lambda'_m)} \right)^{-\lambda'_m} \\
&= 1.
\end{aligned}$$

Hence we obtain the bound

$$e^2_{\mathrm{per},p^m,d_{\max},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \leq e^2_{\mathrm{per},p^m,d_{\max},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(m)}) \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d_{\max},\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d_{\max},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{\alpha}$$

for all $m = m_1, \ldots, m_2$, where $\boldsymbol{z}^*$ is constructed by Algorithm 5 based on the quality measure $F'_{m_1,m_2,d+1,\alpha,\gamma}(z_{d+1})$ with the constant c_m given by (5.15). This shows that the error criteria used in [4] has to satisfy the bound

$$V_{p,m_1,m_2,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \leq \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{\alpha}$$

for $d = 1, \ldots, d_{\max}$.

The values $\lambda'_{m_1}, \ldots, \lambda'_{m_2}$ do not have any influence on the algorithm as seen above, they only appear in the bound above. Hence we have the following result.

Theorem 5.3.9 *Let $d_{\max}$ be positive integer, p prime and $0 < m_1 \leq m_2$. Let c_m be given by (5.15) for all $m = m_1, \ldots, m_2$. Then the modification of Algorithm 5 proposed above, or equivalently the construction algorithm used in [4], constructs a vector $\boldsymbol{z}^* \in \mathcal{Z}_p^d$ such that*

$$V_{p,m_1,m_2,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d^*) \leq \min_{1/\alpha < \lambda'_{m_1}, \ldots, \lambda'_{m_2} \leq 1} \left(\sum_{k=m_1}^{m_2} \left(\frac{\overline{M}^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\lambda'_k)}{e^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})} \right)^{\lambda'_k} \right)^{\alpha}$$

for $d = 1, \ldots, d_{\max}$.

Compared with the numerical results in [4], the bound is certainly conservative. Further, the bound also depends on m_1 and m_2 as each summand in the sum in the bound above is at least 1.

Note that in the theory above we could also use the bound from [8, Theorem 6] instead of $\overline{M}^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\lambda'_k)$, which states that the error is bounded by

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*_d) \leq \frac{C^\alpha (\log\log n)^\alpha}{n^\alpha} \prod_{j=1}^{d} \Big(1 + 2\gamma_j^{1/\alpha}(1 - \log 2 + \zeta(\alpha)^{1/\alpha} + \log n)\Big)^\alpha$$

for all $n \in \mathbb{N}$ (we just used the fact that there is a constant C such that $\phi(n)^{-1} < C(\log\log n)/n$, see for example [20, Theorem 328]). If we use the lower bound from [50] instead of $e^2_{\mathrm{per},p^k,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{(k)})$ we obtain that the bound in Theorem 5.3.9 is at most of order m_2 to some power. Hence also for the algorithm of [4] the worst-case error for the extensible lattice rule can only be worse by a factor of m_2 to some power compared to the worst-case error for a lattice rule constructed by a component-by-component algorithm only for a fixed value of number of points.

5.4 Numerical testing

We have shown that it is possible to construct a generating vector $\boldsymbol{z}^*$ such that

$$e^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*) \leq c_m^{1/\lambda} \overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $\lambda \in (1/\alpha, 1]$ where $c_m \geq 1$ for $m = m_1, \ldots, m_2$ such that $\sum_{m=m_1}^{m_2} c_m^{-1} \leq 1$. The testing was all performed using the fast CBC algorithm since it is the fastest computationally. There are several parameters for each calculation which we must choose. In each example we take $p = \alpha = 2$. We also assume that the constants c_m for $m = m_1, \ldots, m_2$ are equal for each m, that is $c_m = m_2 - m_1 + 1$. For these experiments we take $m_1 = 10$, $m_2 = 20$ and $d_{\max} = 360$.

There are two conclusions which can be drawn from our numerical experiments. The first conclusion we may draw is that the worst-case error for

	$e_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$	$c_m^{1/2\lambda^*}\overline{M}_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\lambda^*)$	$U_{2,10,20,360,2,\boldsymbol{\gamma}}$
$m = 10$	8.20e-02	1.44e+00	5.71e-02
$m = 11$	5.33e-02	1.01e+00	5.25e-02
$m = 12$	3.41e-02	7.17e-01	4.76e-02
$m = 13$	2.21e-02	5.07e-01	4.37e-02
$m = 14$	1.44e-02	3.59e-01	4.00e-02
$m = 15$	9.41e-03	2.54e-01	3.71e-02
$m = 16$	5.81e-03	1.79e-01	3.24e-02
$m = 17$	3.73e-03	1.27e-01	2.94e-02
$m = 18$	2.37e-03	8.97e-02	2.65e-02
$m = 19$	1.53e-03	6.34e-02	2.41e-02
$m = 20$	9.89e-04	4.48e-02	2.20e-02

Table 5.1: Worst-case error of the extensible lattice rule where $\gamma_j = 1/j^2$

the extensible lattice rule is much smaller than the bound in Theorem 5.3.7 suggests. To demonstrate this we define the quantity

$$U_{p,m_1,m_2,d_{\max},\alpha,\boldsymbol{\gamma}} = \max_{1\le d\le d_{\max}} \frac{e_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^{*(m_1,m_2)})}{c_m^{1/2\lambda^*}\overline{M}_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda^*)} \tag{5.16}$$

where $c_m^{1/\lambda^*}\overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda^*) \le c_m^{1/\lambda}\overline{M}^2_{\mathrm{per},p^m,d,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $\lambda \in (1/\alpha, 1]$ and the vector $\boldsymbol{z}^{*(m_1,m_2)}$ is a generating vector constructed with Algorithm 5. Theorem 5.3.7 shows that $U_{p,m_1,m_2,d_{\max},\alpha,\boldsymbol{\gamma}}$ is bounded by 1.

In Tables 5.1–5.3 we compare the values of $U_{2,10,20,360,2,\boldsymbol{\gamma}}$ for different choices of $\boldsymbol{\gamma}$. We see that in each case $U_{2,10,20,360,2,\boldsymbol{\gamma}}$ is orders of magnitude less than 1. In fact, the numerical tests do not find any examples where $U_{2,10,20,360,2,\boldsymbol{\gamma}}$ is greater than 0.062.

The second conclusion we may draw is that the worst-case error for the extensible lattice rule is not significantly greater than the worst-case error for the "near optimal" lattice rule as constructed by the CBC algorithm. To demonstrate this we examine the error measure $V_{p,m_1,m_2,s,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$ defined above.

	$e_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$	$c_m^{1/2\lambda^*}\overline{M}_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\lambda^*)$	$U_{2,10,20,360,2,\boldsymbol{\gamma}}$
$m = 10$	4.00e+02	3.50e+05	5.55e-02
$m = 11$	2.83e+02	2.47e+05	5.04e-02
$m = 12$	2.00e+02	1.75e+05	4.63e-02
$m = 13$	1.41e+02	1.24e+05	4.20e-02
$m = 14$	9.99e+01	8.75e+04	4.23e-02
$m = 15$	7.06e+01	6.18e+04	3.55e-02
$m = 16$	5.00e+01	4.37e+04	3.25e-02
$m = 17$	3.53e+01	3.09e+04	2.95e-02
$m = 18$	2.50e+01	2.19e+04	2.76e-02
$m = 19$	1.77e+01	1.55e+04	2.42e-02
$m = 20$	1.25e+01	1.09e+04	2.27e-02

Table 5.2: Worst-case error of the extensible lattice rule where $\gamma_j = 0.9^j$

	$e_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\boldsymbol{z}^*)$	$c_m^{1/2\lambda^*}\overline{M}_{\mathrm{per},2^m,360,2,\boldsymbol{\gamma}}(\lambda^*)$	$U_{2,10,20,360,2,\boldsymbol{\gamma}}$
$m = 10$	2.51e+10	1.80e+21	6.19e-02
$m = 11$	1.77e+10	1.27e+21	5.85e-02
$m = 12$	1.25e+10	9.01e+20	5.58e-02
$m = 13$	8.87e+09	6.37e+20	5.09e-02
$m = 14$	6.27e+09	4.51e+20	4.85e-02
$m = 15$	4.44e+09	3.19e+20	4.46e-02
$m = 16$	3.14e+09	2.25e+20	4.23e-02
$m = 17$	2.22e+09	1.59e+20	4.04e-02
$m = 18$	1.57e+09	1.13e+20	3.74e-02
$m = 19$	1.11e+09	7.96e+19	3.56e-02
$m = 20$	7.84e+08	5.63e+19	3.43e-02

Table 5.3: Worst-case error of the extensible lattice rule where $\gamma_j = 0.05$

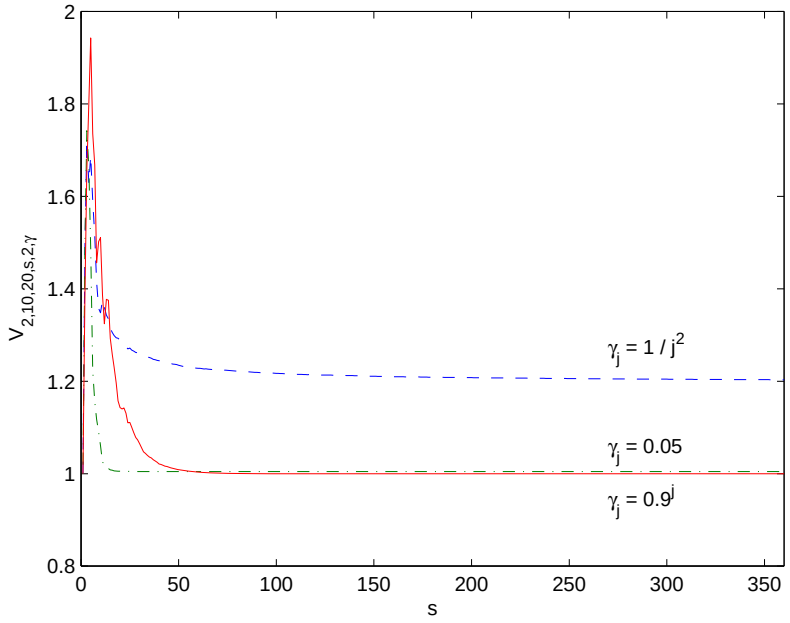

Figure 5.1: Graph of $V_{2,10,20,s,2,\boldsymbol{\gamma}}$ for 3 choices of $\boldsymbol{\gamma}$ and $s = 1, \ldots, 360$

In Figure 5.1 we see when $m_1 = 10$, $m_2 = 20$ and $p = \alpha = 2$ the greatest ratio of the worst-case error of the extensible lattice $\boldsymbol{z}^*$ and the worst-case error of the corresponding near optimal choice $\boldsymbol{z}^{(m)}$ (as constructed by the CBC algorithm) is always less than 2 for these particular choices of $\boldsymbol{\gamma}$. This is similar to the results in [4, Table 6.1].

5.5 Discussion

Though we provide some useful constructions here there are still some open questions. First let us address the meaning of "extensible". In the introduction we wrote that the existence of good extensible lattice rules was shown in [26]. The use of the word "extensible" means that there exists a generating vector $\boldsymbol{z}^*$ such that one can obtain good lattice rules for all moduli $p, p^2, \ldots$. What would be an interesting result in this direction, but was not shown in [26], is the following:

For any generating vector of a good lattice rule in dimension s with number of points p^m, there exists an extension of this generating vector such that one obtains a good lattice rule for some other number of points $p^{m'}$ with $m' \neq m$.

(Compare this statement with a probabilistic version in Remark 5.2.4. Further, an analogous result for the dimension is known if $s' > s$, see [8, 35].) Such a result would indeed be interesting, but at present it is not even known whether this statement is true, let alone how it can be made constructive. This seems to be a much more challenging question as the probabilistic arguments used in [7, 26, 43] and here do not seem to apply, rather one would have to find some number theoretic reason to prove such a result (a constructive algorithm which achieves this might be even more difficult to obtain). Hence in terms of construction, what is known until now is only the existence of good "embedded" lattice rules (embedded in the number of points n), i.e. lattice rules which work well for a whole range of moduli, rather than are extensible. Hence the algorithms introduced here are feasible constructions of good lattice rules achieving what is known until now about their existence. Thus everything known about the existence of extensible lattice rules has been made practical in this paper (see [7] for the analogue for polynomial lattice rules).

To make even more precise what we mean here let us give an example of true extensibility. Namely using the CBC algorithm good lattice rules are truly extensible in the dimension, that is, if one is given a good extensible lattice rule in some finite dimension d then one can add another coordinate to obtain a good lattice rule in $d+1$ dimensions [8, 35, 52]. On the other hand such a lattice rule does not have to be embedded in the dimension: for example, construct a good Korobov lattice rule in dimension d (i.e., the generating vector is of the form $(1, z, z^2, \ldots, z^{d-1})$), then using the CBC algorithm we can add arbitrarily many coordinates to obtain a good lattice rule in $d' > d$ dimensions [15]. But until now we cannot prove that we can extract an $d-1$ dimensional good lattice rule from the d' dimensional or d dimensional lattice rule given at the beginning. Hence our lattice rule is extensible in the dimension, but

not necessarily embedded (meaning that we can extract a good lattice rule from a given one in dimensions $d = 1, 2, 3, \ldots$). Using the CBC algorithm from dimension one onwards we can of course obtain a lattice rule which is extensible and embedded in the dimension in this sense.

Thus, in this terminology, what was shown in [26] is the existence of a good lattice rule which is embedded in n and d simultaneously and this has been made constructive in this paper. Note that in this paper we even improved this result by showing the existence of a lattice rule which is embedded in n and extensible and embedded in d and this is also made constructive in our algorithms (which is achieved by incorporating the CBC approach).

Chapter 6

Korobov-form generating vector extensible in the dimension

In Section 2.6.1 we introduced the Korobov-form generating vector, which is a generating vector of the form

$$\boldsymbol{z}_d(a) = (1, a, a^2, \ldots, a^{d-1}) \pmod{n},$$

where n is prime and a chosen from the set $\mathcal{Z}_{n,1} = \{1, 2, \ldots, n-1\}$. As mentioned in (2.43), it is possible to find an element $a \in \mathcal{Z}_{n,1}$, and hence a generating vector $\boldsymbol{z}_d(a)$ such that

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda), \tag{2.43$'$}$$

where

$$\widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) = (n-1)^{-1/\lambda} d^{1/\lambda} \prod_{j=1}^{d} \left(1 + 2\left(\frac{\gamma_j}{2\pi^2}\right)^{\lambda} \zeta(\alpha\lambda)\right)^{1/\lambda}.$$

As discussed in Section 2.6.1 a major weakness of the Korobov-form vector over other construction approaches such as the CBC algorithm, is that the generating vector $\boldsymbol{z}_d(a)$ is not extensible in dimension. That is, the quantity $e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a))$ is *small* only for fixed d.

In this chapter, we incorporate the ideas of Chapter 5 to derive an algorithm to construct a generating vector of the Korobov form which is good for a range

of dimensions. The existence of extensible Korobov-form rules was first shown for polynomial lattice rules by Niederreiter [43].

6.1 Construction of extensible rules

In this section, we shall demonstrate how to choose an element $a \in \mathcal{Z}_{n,1}$ such that for a given set $\mathcal{S} = \{d_1, \ldots, d_s\}$, and corresponding set of positive constants $c_1, \ldots, c_s$, for each $k = 1, \ldots, d$

$$e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \le c_k^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda) \tag{6.1}$$

for all $\lambda \in (1/\alpha, 1]$.

Let μ be the equiprobable measure on the set $\mathcal{Z}_{n,1}$. For a real $c \ge 1$ we define the set

$$\mathcal{C}_{n,d,\alpha,\boldsymbol{\gamma}}(c) = \left\{ a \in \mathcal{Z}_{n,1} \,:\, e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \le c \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}} \right\}.$$

In the subsequent theorem we give a lower bound on the measure of this set.

Theorem 6.1.1 *Let $\alpha > 1$, n prime and d be a positive integer. Then for any $c \ge 1$ we have $\mu(\mathcal{C}_{n,d,\alpha,\boldsymbol{\gamma}}(c)) > 1 - c^{-1}$.*

Proof. This follows immediately from applying Markov's inequality to (2.43′) with $\lambda = 1$. □

Furthermore, for a real $c \ge 1$ we define the set

$$\widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c) = \Big\{ a \in \mathcal{Z}_{n,1} \,:\, e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \le c^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda) \quad \text{for all } \lambda \in (1/\alpha, 1] \Big\}.$$

We obtain the following theorem.

Theorem 6.1.2 *Let $\alpha > 1$, n prime and d be a positive integer. Then for any $c \ge 1$ we have $\mu\left(\widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c)\right) > 1 - c^{-1}$.*

Proof. The proof of this theorem is almost identical to that of Theorem 5.2.2. □

To find a generating vector of the Korobov form such that (6.1) is satisfied, we seek an element $a \in \mathcal{Z}_{n,1}$ such that

$$a \in \bigcap_{d \in \mathcal{S}} \widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c_d).$$

In the theorem below, we see this is possible if we choose $c_d \geq 1$ large enough such that $\sum_{d \in \mathcal{S}} c_d^{-1} \leq 1$.

Theorem 6.1.3 *Let $\alpha > 1$, n prime and $\mathcal{S}$ be a subset of $\mathbb{N}$. Let $c_d \geq 1$ for all $d \in \mathcal{S}$, such that $\sum_{d \in \mathcal{S}} c_s^{-1} \leq 1$. Then there exists an $a \in \mathcal{Z}_{n,1}$ such that*

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq c_d^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $d \in \mathcal{S}$ and all $\lambda \in (1/\alpha, 1]$.

Proof. As

$$\begin{aligned}\mu\left(\bigcap_{d \in \mathcal{S}} \widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c_d)\right) &= 1 - \mu\left(\bigcup_{d \in \mathcal{S}} \widetilde{\mathcal{C}}^c_{n,d,\alpha,\boldsymbol{\gamma}}(c_d)\right) \\ &\geq 1 - \sum_{d \in \mathcal{S}} \mu(\widetilde{\mathcal{C}}^c_{n,d,\alpha,\boldsymbol{\gamma}}(c_d)) > 1 - \sum_{d \in \mathcal{S}} c_d^{-1} \geq 0,\end{aligned}$$

by Lemma 6.1.2 and our assumption on the choice of c_d, it follows that the set $\bigcap_{d \in \mathcal{S}} \widetilde{\mathcal{C}}_{n,d,\alpha,\boldsymbol{\gamma}}(c_d)$ is not empty and we are done. □

Remark 6.1.4 Note that it is always possible to choose c_d of order $d^{1+\varepsilon}$ for some $\varepsilon > 0$. Hence the factor $c_d^{1/\lambda}$ in the above bound can be chosen such that it contributes at most another factor of $d^{(1+\varepsilon)/\lambda}$.

Assuming the conditions of Theorem 6.1.3, using Algorithm 6 one can find generating vectors of Korobov form for which the worst-case error satisfies the bound from Theorem 6.1.3 for a given set of dimensions.

Algorithm 6 Search for $a \in \mathcal{Z}_{n,1}$ with small $e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a))$ for all $d \in \mathcal{S}$

Require: $\mathcal{S} = \{d_1, \ldots, d_s\}$, $\alpha > 1$, a positive sequence of weights $\boldsymbol{\gamma}$, n prime and the positive sequence $c_{d_1}, \ldots, c_{d_s} \geq 1$ such that $\sum_{d \in \mathcal{S}} c_d^{-1} \leq 1$.

1: $T_0 = \mathcal{Z}_{n,1}$.

2: **for** $k = 1$ to s **do**

3: Find at least $\lfloor (1 - \sum_{i=1}^{k} c_{d_i}^{-1})(n-1) \rfloor + 1$ elements to populate the set

$$T_k \subseteq \{a \in T_{k-1} : e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \leq c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda), \text{ for all } \lambda \in (1/\alpha, 1]\}.$$

4: **end for**

5: Choose any $a \in T_s$.

Theorem 6.1.5 *Let $\alpha > 1$, n prime and $\mathcal{S}$ be a subset of $\mathbb{N}$. Let $c_d \geq 1$ for all $d \in \mathcal{S}$, such that $\sum_{d \in \mathcal{S}} c_d^{-1} \leq 1$. Then Algorithm 6 gives an element $a \in \mathcal{Z}_{n,1}$ such that*

$$e^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a)) \leq c_d^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda)$$

for all $d \in \mathcal{S}$ and all $\lambda \in (1/\alpha, 1]$.

Proof. Let $\mathcal{S} = \{d_1, \ldots, d_s\}$. We show by induction on d that the sets T_{k-1}, as constructed by Algorithm 6, contain at least $\lfloor (1 - \sum_{i=1}^{k} c_{d_i}^{-1})(n-1) \rfloor + 1$ elements a such that $e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \leq c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda)$ for all $1 \leq k \leq d$ and all $\lambda \in (1/\alpha, 1]$.

Assume that $c_{d_1}^{-1} \leq 1$. Then it follows from Lemma 6.1.2 that there are at least $\lfloor (1 - c_{d_1}^{-1})(n-1) \rfloor + 1$ elements $a \in \mathcal{Z}_{n,1} = T_0$ such that

$$e^2_{\mathrm{per},n,d_1,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_1}(a)) \leq c_{d_1}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_1,\alpha,\boldsymbol{\gamma}}(\lambda).$$

Hence the result is proved for $k = 1$.

Assume now that $\sum_{i=1}^{k+1} c_{d_i}^{-1} \leq 1$ and that for some integer $1 \leq k < s$ we have at least $\lfloor (1 - \sum_{i=1}^{k} c_{d_i}^{-1})(n-1) \rfloor + 1$ elements in the set

$$\{a \in T_{k-1} : e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \leq c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\},$$

that is,

$$\mu\left(\{a \in T_{k-1} : e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \le c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}\right)$$
$$> \ 1 - \sum_{i=1}^{k} c_{d_i}^{-1}.$$

We show that

$$\mu\left(\{a \in T_k : e^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_{k+1}}(a)) \le c_{d_{k+1}} \widehat{M}^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}\right)$$
$$> \ 1 - \sum_{i=1}^{k+1} c_{d_i}^{-1},$$

from which the result then follows as $1 - \sum_{i=1}^{k+1} c_{d_i}^{-1} \ge 0$ and hence the above set is not empty. We have

$$\{a \in T_k : e^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_{k+1}}(a)) \le c_{d_{k+1}}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}$$
$$= \{a \in T_{k-1} : e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \le c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}$$
$$\cap\ \{a \in \mathscr{Z}_{n,1} : e^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{s_{k+1}}(a)) \le c_{d_{k+1}}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}.$$

Hence

$$\mu\left(\{a \in T_k : e^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_{k+1}}(a)) \le c_{d_{k+1}}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}\right)$$
$$= 1 - \mu\Big(\{a \in T_{k-1} : e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a)) \le c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}^c$$
$$\cup\ \{a \in \mathscr{Z}_{n,1} : e^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_{k+1}}(a)) \le c_{d_{k+1}}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_{k+1},\alpha,\boldsymbol{\gamma}}(\lambda),\ \forall\, \lambda \in (1/\alpha, 1]\}^c\Big)$$
$$\ge 1 - \left(\sum_{i=1}^{k} c_{d_i}^{-1} + c_{d_{k+1}}^{-1}\right)$$
$$= 1 - \sum_{i=1}^{k+1} c_{d_i}^{-1},$$

where we used the induction hypothesis and Lemma 6.1.2. The result follows. □

6.2 Numerical results

In this section we examine the quality of the Korobov-form generating vectors which are good for multiple values of d. The experiment we perform constructs

a generating vector of extensible Korobov form with small worst-case error for each $d \in \mathcal{S}$ where $\mathcal{S} = \{5, 10, 25, 50, 100\}$. We compare this worst-case error with the bound achieved in Theorem 6.1.5 and with the worst-case error of the non-extensible Korobov rule. Further, we compare the worst-case error with the worst-case error of the generating vector constructed by the CBC algorithm. Each comparison is made for different values of prime n and different sets of weights $\boldsymbol{\gamma}$. In our experiments we have chosen $\alpha = 2$.

Tables 6.1 and 6.2 contain the results of these experiments. The rows marked "Bound" contain the quantity

$$\min_{1/\alpha<\lambda\leq 1} c_d^{1/(2\lambda)} \widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\lambda),$$

where $\widehat{M}^2_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}$ is a bound on the root mean square worst-case error. The rows marked "Ext. Korobov" contain the root mean square worst-case error $e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a))$ in the weighted Korobov space, and where a is constructed by Algorithm 6. The rows marked "Korobov" contain the root mean square worst-case error $e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_d(a))$, where a is chosen to have the smallest root mean square worst-case error for that particular choice of d. Finally, the row marked "CBC" contains the root mean square worst-case error $e_{\mathrm{per},n,d,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z})$, where the generating vector $\boldsymbol{z}$ is chosen using the CBC algorithm. The choice of $a \in T_s$ in Line 5 of Algorithm 6 is taken to be

$$\operatorname*{argmin}_{a\in T_s} \sum_{k=1}^{s} \frac{e^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{d_k}(a))}{c_{d_k}^{1/\lambda^*} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda^*)}$$

where $1/\alpha < \lambda^* \leq 1$ is the minimiser of $c_{d_k}^{1/\lambda} \widehat{M}^2_{\mathrm{per},n,d_k,\alpha,\boldsymbol{\gamma}}(\lambda)$. The constants c_{d_k} are all taken to be 5.

The first observation we can make from the results in Tables 6.1 and 6.2 is that the extensible Korobov rule has a worst-case error much smaller than the bound in Theorem 6.1.5 suggests. This is similar to the results observed in [61]. The second observation we may make is that the worst-case error for the extensible Korobov rule is not much greater than that of either the Korobov rule for fixed dimension or the lattice rule constructed using the CBC

n	Method	$d = 5$	$d = 10$	$d = 25$	$d = 50$	$d = 100$
257	Bound	3.36e-01	4.99e-01	7.93e-01	1.12e+00	1.59e+00
	Ext. Korobov	3.03e-03	3.71e-03	4.24e-03	4.51e-03	4.68e-03
	Korobov	3.03e-03	3.68e-03	4.24e-03	4.51e-03	4.68e-03
	CBC	2.88e-03	3.27e-03	3.60e-03	3.75e-03	3.83e-03
509	Bound	2.24e-01	3.45e-01	5.63e-01	7.98e-01	1.13e+00
	Ext. Korobov	1.52e-03	1.83e-03	2.71e-03	2.87e-03	2.93e-03
	Korobov	1.52e-03	1.83e-03	2.40e-03	2.59e-03	2.68e-03
	CBC	1.50e-03	1.72e-03	1.91e-03	2.00e-03	2.06e-03
1021	Bound	1.46e-01	2.32e-01	3.93e-01	5.63e-01	7.97e-01
	Ext. Korobov	8.48e-04	1.22e-03	1.59e-03	1.66e-03	1.78e-03
	Korobov	8.48e-04	1.07e-03	1.31e-03	1.50e-03	1.61e-03
	CBC	7.83e-04	9.14e-04	1.03e-03	1.08e-03	1.11e-03
2053	Bound	9.27e-02	1.52e-01	2.68e-01	3.93e-01	5.62e-01
	Ext. Korobov	4.30e-04	6.47e-04	8.14e-04	8.92e-04	9.23e-04
	Korobov	4.30e-04	5.75e-04	6.81e-04	7.71e-04	8.51e-04
	CBC	4.05e-04	4.81e-04	5.46e-04	5.76e-04	5.95e-04

Table 6.1: Comparison table for classical lattice rules with $\gamma_j = 1/j^2$

algorithm. Hence from a practical point of view we obtain Korobov lattice rules which are useful for a range of dimensions.

n	Method	$d = 5$	$d = 10$	$d = 25$	$d = 50$	$d = 100$
257	Bound	4.17e-01	7.03e-01	1.36e+00	2.03e+00	2.88e+00
	Ext. Korobov	1.12e-02	2.66e-02	5.19e-02	6.00e-02	6.08e-02
	Korobov	1.12e-02	2.58e-02	5.19e-02	6.00e-02	6.08e-02
	CBC	1.02e-02	2.45e-02	5.02e-02	5.80e-02	5.86e-02
509	Bound	2.96e-01	4.99e-01	9.68e-01	1.44e+00	2.04e+00
	Ext. Korobov	7.90e-03	1.74e-02	3.34e-02	3.95e-02	4.00e-02
	Korobov	5.92e-03	1.59e-02	3.34e-02	3.93e-02	3.98e-02
	CBC	5.78e-03	1.51e-02	3.19e-02	3.73e-02	3.77e-02
1021	Bound	2.07e-01	3.52e-01	6.83e-01	1.02e+00	1.44e+00
	Ext. Korobov	4.67e-03	1.05e-02	2.19e-02	2.65e-02	2.68e-02
	Korobov	3.45e-03	9.69e-03	2.19e-02	2.61e-02	2.65e-02
	CBC	3.31e-03	9.01e-03	2.01e-02	2.37e-02	2.40e-02
2053	Bound	1.42e-01	2.48e-01	4.82e-01	7.16e-01	1.02e+00
	Ext. Korobov	3.34e-03	6.20e-03	1.33e-02	1.58e-02	1.77e-02
	Korobov	1.93e-03	5.76e-03	1.33e-02	1.58e-02	1.66e-02
	CBC	1.78e-03	5.37e-03	1.27e-02	1.51e-02	1.53e-02

Table 6.2: Comparison table for classical lattice rules with $\gamma_j = 0.9^j$

n	Method	$d = 5$	$d = 10$	$d = 25$	$d = 50$	$d = 100$
257	Bound	2.57e-01	4.43e-01	7.75e-01	1.22e+00	2.12e+00
	Ext. Korobov	1.09e-03	1.99e-03	5.37e-03	1.37e-02	3.52e-02
	Korobov	9.31e-04	1.74e-03	5.04e-03	1.32e-02	3.52e-02
	CBC	9.29e-04	1.70e-03	5.27e-03	1.36e-02	3.53e-02
509	Bound	1.60e-01	2.95e-01	5.50e-01	8.63e-01	1.50e+00
	Ext. Korobov	7.16e-04	1.47e-03	4.11e-03	8.73e-03	2.17e-02
	Korobov	4.66e-04	9.10e-04	3.00e-03	8.00e-03	2.17e-02
	CBC	4.68e-04	8.75e-04	3.05e-03	8.09e-03	2.23e-02
1021	Bound	9.76e-02	1.92e-01	3.87e-01	6.09e-01	1.06e+00
	Ext. Korobov	4.31e-04	1.01e-03	2.54e-03	5.57e-03	1.36e-02
	Korobov	2.44e-04	5.02e-04	1.71e-03	4.90e-03	1.36e-02
	CBC	2.43e-04	4.73e-04	1.69e-03	4.75e-03	1.38e-02
2053	Bound	5.86e-02	1.23e-01	2.67e-01	4.30e-01	7.48e-01
	Ext. Korobov	1.36e-04	2.64e-04	1.14e-03	3.08e-03	8.72e-03
	Korobov	1.23e-04	2.64e-04	9.49e-04	2.84e-03	8.72e-03
	CBC	1.23e-04	2.49e-04	9.27e-04	2.88e-03	8.73e-03

Table 6.3: Comparison table for classical lattice rules with $\gamma_j = 0.05$

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