Construction of lattice rules for multiple integration based on a weighted discrepancy

A thesis

submitted in fulfilment

of the requirements for the Degree

of

Doctor of Philosophy

at the

University of Waikato

by

Vasile Sinescu

THE UNIVERSITY OF
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Te Whare Wānanga o Waikato

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Abstract

High-dimensional integrals arise in a variety of areas, including quantum physics, the physics and chemistry of molecules, statistical mechanics and more recently, in financial applications.

In order to approximate multidimensional integrals, one may use Monte Carlo methods in which the quadrature points are generated randomly or quasi-Monte Carlo methods, in which points are generated deterministically. One particular class of quasi-Monte Carlo methods for multivariate integration is represented by lattice rules. Lattice rules constructed throughout this thesis allow good approximations to integrals of functions belonging to certain weighted function spaces. These function spaces were proposed as an explanation as to why integrals in many variables appear to be successfully approximated although the standard theory indicates that the number of quadrature points required for reasonable accuracy would be astronomical because of the large number of variables.

The purpose of this thesis is to contribute to theoretical results regarding the construction of lattice rules for multiple integration. We consider both lattice rules for integrals over the unit cube and lattice rules suitable for integrals over Euclidean space. The research reported throughout the thesis is devoted to finding the generating vector required to produce lattice rules that have what is termed a "low weighted discrepancy". In simple terms, the "discrepancy" is a measure of the uniformity of the distribution of the quadrature points or in other settings, a worst-case error. One of the assumptions used in these weighted function spaces is that variables are arranged in the decreasing order of their importance and the assignment of weights in this situation results in so-called "product weights". In other applications it is rather the importance of group of variables that matters. This situation is modelled by using function spaces in which the weights are "general". In the weighted settings mentioned above, the quality of the lattice rules is assessed by the "weighted discrepancy" mentioned earlier. Under appropriate conditions on the weights, the lattice rules constructed here produce a convergence rate of the error that ranges from $O(n^{-1/2})$ to the (believed) optimal $O(n^{-1+\delta})$ for any $\delta > 0$, with the involved constant independent of the dimension.

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First, I would like to thank and express my deepest gratitude to Associate Professor Stephen Joe, without whom this thesis wouldn't have been possible. Stephen has been a great mentor throughout these years and I had to learn a lot from his attitude of approaching research and from his outstanding computer skills. I hope to continue my collaboration with Stephen in the future.

Next, I would like to thank my second supervisor, Dr Rua Murray, for his continuous support and for many useful discussions we've had throughout my doctoral studies. Many thanks also to Associate Professor Kevin Broughan who has enlightened me on several Number Theory results.

My acknowledgements extend to the whole Department of Mathematics and to the University of Waikato for offering me the doctoral scholarship. I would also like to thank the New Zealand Mathematical Society for providing me some financial support that helped me travel to conferences in Germany and Romania.

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Contents

Chapter 1

Introduction

1.1 Lattice rules for numerical multiple integration

Integrals over the d-dimensional unit cube given by

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

may be approximated by quadrature rules of the form

$$Q_{n,d}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f(\boldsymbol{t}_k). \tag{1.2}$$

If the quadrature points $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1} \in [0,1)^d$ are produced in some deterministic manner, then the quadrature rule (1.2) is known as a quasi-Monte Carlo rule for numerical multiple integration. A particular class of quasi-Monte Carlo methods is represented by lattice rules. Quasi-Monte Carlo methods in general and lattice rules in particular, have recently become of more interest especially due to their efficiency in applications arising from mathematical finance (see [45]). We start by revising some aspects of the definition and the theory of lattice rules that will be used throughout the thesis. In-depth details can be found in [51].

In Mathematics the notion of "lattice" has several meanings. Throughout this thesis, the concepts of "lattice", "integration lattice", and "lattice rule" are defined as follows:

Definition 1.1 *By a d-dimensional lattice, we mean a discrete set of points in $\mathbb{R}^d$ which is closed under addition and subtraction.*

Definition 1.2 *An integration lattice is a lattice that contains $\mathbb{Z}^d$ as a subset.*

Definition 1.3 *A lattice rule is a quadrature rule of the form* (1.2) *whose quadrature points are all the points of an integration lattice that lie in the half-open unit cube $[0,1)^d$.*

It has been established in [53] that every lattice rule can be written in the so-called "canonical form" as a multiple sum of the form

$$Q_{n,d}(f) = \frac{1}{n} \sum_{k_1=0}^{n_1-1} \sum_{k_2=0}^{n_2-1} \cdots \sum_{k_r=0}^{n_r-1} f\left(\left\{ \frac{k_1 \boldsymbol{z}_1}{n_1} + \frac{k_2 \boldsymbol{z}_2}{n_2} + \cdots \frac{k_r \boldsymbol{z}_r}{n_r} \right\} \right), \tag{1.3}$$

where $n = n_1 \cdots n_r$ with $n_{i+1} | n_i$ for every $1 \le i \le r-1$ and $\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots, \boldsymbol{z}_r$ are linearly independent integer vectors such that each vector $\boldsymbol{z}_i$ has no factor in common with n_i for every $1 \le i \le r$. In the canonical form (1.3), r is known as the "rank" of the lattice rule and represents the minimal number of sums required to write it down. In (1.3) and throughout the whole thesis, the braces around a vector indicate that we take the fractional part of each component of the vector. The canonical form of a lattice rule is not necessarily the most convenient in practice. For instance, the intermediate-rank lattice rules defined by (1.7) (see below) and studied in Chapter 3 are not written in canonical form.

Apart from integrals of the form (1.1), in this thesis we also consider weighted integrals over Euclidean space defined by

$$I_d(f, \rho) = \int_{\mathbb{R}^d} f(\boldsymbol{x}) \rho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}, \tag{1.4}$$

where the weight function $\rho(\boldsymbol{x})$ is a probability density. Hence $\rho(\boldsymbol{x}) \ge 0$ for any $\boldsymbol{x} \in \mathbb{R}^d$ and $\int_{\mathbb{R}^d} \rho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 1$. Such integrals may also be approximated by quasi-Monte Carlo rules of the form (1.2). As we shall see later, these integrals are first transformed to equivalent integrals over the unit cube.

1.1.1 Rank-1 lattice rules

When a lattice rule may be written by using a single sum ($r = 1$ in the representation (1.3)), then we obtain a rank-1 lattice rule, whose form is given by

$$Q_{n,d}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\boldsymbol{z}}{n}\right\}\right), \tag{1.5}$$

where $\boldsymbol{z}$ is usually named the "generating vector" of the lattice rule. Usually, the generating vector is restricted to the set $\mathcal{Z}_n^d$, where $\mathcal{Z}_n := \{z : z \in \{1, 2, \ldots, n-1\},\ \gcd(z, n) = 1\}$. Obviously, the number of elements of the set $\mathcal{Z}_n$ is given by $|\mathcal{Z}_n| = \varphi(n)$, where φ is Euler's totient function.

We will also consider "shifted rank-1 lattice rules". These are quasi-Monte Carlo rules of the form

$$Q_{n,d}(f, \boldsymbol{\Delta}) = \frac{1}{n}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\boldsymbol{z}}{n} + \boldsymbol{\Delta}\right\}\right), \tag{1.6}$$

where $\boldsymbol{\Delta} \in [0, 1)^d$ is the "shift". Let us remark that the points of a shifted lattice rule do not belong to an integration lattice in the sense of Definition 1.2. As we shall see later, these shifted lattice rules are especially suited to integrals over $\mathbb{R}^d$.

1.1.2 Intermediate-rank lattice rules

In this thesis we will also consider lattice rules obtained by "copying" rank-1 lattice rules. If $\ell \geq 1$ is an integer satisfying $\gcd(\ell, n) = 1$ and r is a fixed integer taken from the set $\{0, 1, \ldots, d\}$, then we can define the following lattice rule:

$$Q_{N,d}^{(r)}(f) = \frac{1}{\ell^r n}\sum_{m_r=0}^{\ell-1} \cdots \sum_{m_1=0}^{\ell-1}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell}\right\}\right). \tag{1.7}$$

If $r = 0$ and/or $\ell = 1$, then (1.7) becomes the rank-1 lattice rule (1.5). For $r \geq 1$, (1.7) is a rank-r lattice rule or "intermediate-rank lattice rule" having $N = \ell^r n$ distinct points. As mentioned earlier, the lattice rule (1.7) is not written in canonical form, since it has rank r but is expressed using $r + 1$

sums. However, such an expression of an intermediate-rank lattice rule is useful for our analysis in Chapter 3.

1.1.3 Korobov-type lattice rules

The first proof of the existence of "good" lattice rules was given by Korobov in [32] in the situation when n is prime (later in our analysis on Korobov lattice rules we make the same assumption). In [32], the generating vector $\boldsymbol{z}$ of a lattice rule (1.5) was restricted to the so-called Korobov form, that is

$$\boldsymbol{z} := (1, a, \ldots, a^{d-1}) \,(\mathrm{mod}\, n), \tag{1.8}$$

where a is a suitable integer chosen from $\mathcal{Z}_n$. The "Korobov-type lattice rules" considered in this thesis are lattice rules of the form (1.5) or (1.7) with the generating vector $\boldsymbol{z}$ of the form (1.8). Korobov's results were later extended by Niederreiter in [41] for any integer $n > 0$. Niederreiter's result implies essentially the existence of "good" lattice rules in the sense of having a bound of $O(n^{-1}(\ln n)^d)$ for the "discrepancy". The concept of "discrepancy" will be introduced in the next section and treated in-depth throughout the thesis.

1.2 Weighted star discrepancy

In order to assess the goodness of a quasi-Monte Carlo method, there are a number of criteria known in the specialised literature. These criteria are discussed in general works on the theory of lattice rules such as [42] and [51]. One such criterion is based on the idea of "discrepancy", which in simple terms assesses the uniformity of the distribution of the quadrature points. In other settings, the "discrepancy" is considered to be a worst-case error in certain function spaces (as in Chapter 6). The concept of local discrepancy of a point set in $[0,1]^d$ can be described as the difference between the proportion of the points that lie in a subset of $[0,1]^d$ and the measure of that subset. More formally, the local star discrepancy can be defined as follows:

Definition 1.4 *Let $P_n = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ be a set of n quadrature points in $[0,1]^d$. Then the local star discrepancy of the point set P_n at $\boldsymbol{x} \in [0,1]^d$ is defined by*

$$\mathrm{discr}(\boldsymbol{x}, P_n) := \frac{|[\boldsymbol{0}, \boldsymbol{x}) \cap P_n|}{n} - \prod_{j=1}^{d} x_j, \tag{1.9}$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)$.

Definition 1.5 *The unweighted star discrepancy of the point set P_n is defined as*

$$D^*(P_n) := \sup_{\boldsymbol{x} \in [0,1]^d} \left|\mathrm{discr}(\boldsymbol{x}, P_n)\right|. \tag{1.10}$$

This is the star discrepancy that arises in connection with the well-known Koksma-Hlawka inequality:

$$\left| \frac{1}{n} \sum_{k=0}^{n-1} f(\boldsymbol{t}_k) - I_d(f) \right| \leq D^*(P_n) V_{HK}(f), \tag{1.11}$$

where $V_{HK}(f)$ is the variation in the sense of Hardy and Krause. More details on the Koksma-Hlawka inequality can be found in [26] and [64] or in more general works such as [34] or [42]. Nevertheless, let us remark that the right-hand-side of (1.11) involves two quantities: one dependent on the point set and independent of the function (the discrepancy) and the second depending on the function but independent of the point set (the variation). In general terms, the research reported in the thesis is focused on the concept of "discrepancy" and the central idea consists of generating lattice rules having a "low weighted discrepancy". The expression of the discrepancy may have different forms depending on the particular settings used in each chapter and these different expressions will be analysed in-depth throughout the thesis.

In integrals such as (1.1) or (1.4), it is possible that variables or groups of variables are of different importance. Such an assumption leads to the idea of a weight associated with a variable or group of variables, which in turn leads to the concept of "weighted discrepancy". Throughout the thesis, we will establish inequalities of the form (1.11), in which the discrepancy from the right-hand-side of (1.11) is replaced by a weighted discrepancy. Below,

we explain briefly the weighted settings considered in the thesis and give an example of a Koksma-Hlawka type inequality.

Let's consider an arbitrary subset $\mathfrak{u}$ of $\mathcal{D} := \{1, 2, \ldots, d\}$ and let's denote by $\boldsymbol{\gamma}_{\mathfrak{u}}$ the weight associated with the set $\mathfrak{u}$. Throughout the whole thesis, the weights are assumed to be non-negative numbers. Such "weights" has been first introduced in [57], where it was assumed that the dependence of functions on successive variables is increasingly limited. Assuming that the variables are ordered so that the j-th variable is the j-th most important, we can consider a sequence of weights $\{\gamma_j\}_{j=1}^{\infty}$ such that $\gamma_1 \geq \gamma_2 \geq \cdots \gamma_j \geq \cdots$. This then leads to

$$\boldsymbol{\gamma}_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j. \tag{1.12}$$

These weights are known as "product weights" and, in [57] it was also assumed that $\gamma_1 = 1$.

In other applications it is the relative importance of distinct group of variables that matters and this leads to the concept of "general weights". Such a model is the so-called "ANOVA decomposition" of functions. The expansion

$$f(\boldsymbol{x}) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} f_{\mathfrak{u}}(\boldsymbol{x})$$

is an ANOVA decomposition of f, where each term is given by

$$f_{\mathfrak{u}}(\boldsymbol{x}) := \int_{[0,1)^{d-|\mathfrak{u}|}} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}_{\mathcal{D}\setminus\mathfrak{u}} - \sum_{\mathfrak{g} \subset \mathfrak{u}} f_{\mathfrak{g}}(\boldsymbol{x}),$$

with the last sum taken over strict subsets of $\mathfrak{u}$. It can then be checked that $f_{\emptyset} = \int_{[0,1)^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$ and that for each $f_{\mathfrak{u}}$, we have $\int_0^1 f_{\mathfrak{u}}(\boldsymbol{x}) \, \mathrm{d}x_j = 0$ if $j \in \mathfrak{u}$. The term "ANOVA" stands for "analysis of variance" and the technique is widely used in statistics and in some financial applications (see [60] for further details). As a simple example, let's consider the function

$$f(x_1, x_2, x_3) = 4x_1^3 + x_2 \cos(\pi x_3).$$

The ANOVA terms of this function are $f_{\emptyset} = 1, f_{\{1\}}(\boldsymbol{x}) = 4x_1^3 - 1, f_{\{3\}}(\boldsymbol{x}) = \cos(\pi x_3)/2, f_{\{2,3\}}(\boldsymbol{x}) = x_2 \cos(\pi x_3) - \cos(\pi x_3)/2$, while all the other terms are zero.

In [60], the authors remarked that functions deriving from finance are often of a low effective dimension in the sense that these functions can be well approximated by their low-order ANOVA terms. In the ANOVA expansion of f, each term $f_{\mathfrak{u}}$ describes the interaction between variables that belong to $\mathfrak{u}$, since it only depends on these variables. Also in [60], the authors observed that the importance of each dimension is naturally weighted. For instance, it might be the case that only interactions between two variables are important, but those involving more than two variables can be ignored. In such a case it is desirable to introduce so-called "general weights" which describe the relative importance of each distinct group of variables.

Throughout the thesis, we will assume that the weights are either "product" or "general", which is in line with the usual assumptions made in the specialised literature (details can be found in many research papers including but not limited to [9], [20], [21], [22], [25], [29], [35], [36], [37], [38], [52], [56], [61], [62] as well as in [48], [49], [50] and [47]). The concept of "weighted star discrepancy" is based on the discrepancy defined by (1.10) and will be discussed in detail during the following chapters. For instance in Chapter 2, our research will be concentrated on the following weighted star discrepancy:

$$D^*_{n,\boldsymbol{\gamma}}(P_n) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} \left|\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_n)\right|,$$

where by $\boldsymbol{x}_{\mathfrak{u}}$ we denote the vector from $[0,1]^{|\mathfrak{u}|}$ containing the components of $\boldsymbol{x}$ whose indices belong to $\mathfrak{u}$, while by $(\boldsymbol{x}_{\mathfrak{u}},\mathbf{1})$ we mean the vector from $[0,1]^d$ whose j-th component is x_j if $j\in\mathfrak{u}$ and 1 if $j\notin\mathfrak{u}$. This weighted star discrepancy will occur in the following Koksma-Hlawka type inequality (see for instance [29] and [48]):

$$\begin{aligned}\left|Q_{n,d}(f)-I_d(f)\right| \;\leq\; & \left(\max_{\mathfrak{u}\subseteq\mathcal{D}} \sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} \boldsymbol{\gamma}_{\mathfrak{u}}\left|\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_n)\right|\right)\\ & \times\left(\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}^{-1}\int_{[0,1]^{|\mathfrak{u}|}}\left|\frac{\partial^{|\mathfrak{u}|}}{\partial\boldsymbol{x}_{\mathfrak{u}}}f((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}))\right|\,\mathrm{d}\boldsymbol{x}_{\mathfrak{u}}\right). \quad (1.13)\end{aligned}$$

As mentioned earlier, further details on this inequality and the associated weighted star discrepancy will be presented in Chapter 2.

1.3 Tractability and strong tractability of numerical multiple integration

In the previous section, we saw that if f is a function with integrable partial mixed first derivatives, then the quadrature error $|Q_{n,d}(f) - I_d(f)|$ produced by a quasi-Monte Carlo rule of the form (1.2) can be bounded by (1.13). We turn our attention now to the concepts of tractability and strong tractability, which have been studied in many research papers. These concepts are based on the minimal number of function evaluations, say $n(\varepsilon)$, required to reduce the initial error by a factor $\varepsilon \in (0, 1)$. By "initial error", we normally mean the true value of the integral, i.e. the error obtained when the function is not sampled. Formally, tractability and strong tractability are defined as follows:

Definition 1.6 *The integration problem is said to be tractable if there exists a quadrature rule of the form* (1.2) *such that* $n(\varepsilon)$ *can be bounded by a polynomial in* ε^{-1} *and* d*, that is* $n(\varepsilon) \leq C\varepsilon^{-p}d^q$ *for some positive constant* C *independent of* d *and* n *and some non-negative* p *and* q*.*

Definition 1.7 *Strong tractability means that* $n(\varepsilon) \leq C\varepsilon^{-p}$ *for some positive constant* C *independent of* d *and* n *and some non-negative* p*.*

p and q are named the ε-exponent and the d-exponent of tractability respectively. If $q = 0$ then the minimal number p satisfying $n(\varepsilon) \leq C\varepsilon^{-p}$ is named the ε-exponent of strong tractability.

In a non-weighted setting all variables have the same importance and this leads to an exponential increase of $n(\varepsilon)$ with the dimension d. This is the so-named "curse of dimensionality" and leads to intractability of the integration problem. By the other hand, we see that if $n(\varepsilon) \leq C\varepsilon^{-p}$ and the constant C is independent of the dimension, then $n(\varepsilon)$ is independent of the dimension and thus the curse of dimensionality is broken.

In this thesis we shall establish sufficient conditions for tractability and strong tractability under certain assumptions. Such conditions on tractabil-

ity/strong tractability in a weighted context have been studied in many research papers including [9], [20], [21], [22], [24], [56], or [57]. The general result we are aiming for, is either to obtain bounds on the discrepancy for which the dependency on the dimension is at most polynomial (this ensures tractability), or bounds on the discrepancy that are independent of the dimension. The latter ensures strong tractability of the integration problem.

1.4 The structure of the thesis

Throughout the thesis, we construct lattice rules for the approximation of integrals given by (1.1) and (1.4). The generating vector of these lattice rules may be constructed by using the so-called "component-by-component" (CBC) technique and this technique will be used except of Chapter 4, where we consider Korobov-type lattice rules. The CBC technique is essentially a "greedy"-type algorithm in which each component is obtained after successive 1-dimensional searches. Basically, the generating vector in dimension, say $d+1$, will be obtained without altering the first existing d-components. At each step $m = 1, 2, \ldots, d$, the value chosen for the component z_m will be the one that minimises a certain measure of error.

The thesis establishes results of a theoretical nature and as a whole, may be divided into two major parts. Chapters 2–5 are dedicated to lattice rules for integrals over the unit cube given by (1.1), while in Chapters 6–7 we study lattice rules suitable for integrals over Euclidean space given by (1.4).

In general, every chapter is built up on a template that can be described as follows:

- First, we express the error either via a Koksma-Hlawka type inequality (Chapters 2–5 and 7) or as a worst-case error in a reproducing kernel Hilbert space (Chapter 6).

- Then we define a certain weighted discrepancy. Since weighted discrepancies are in general very hard to compute, we instead consider upper

bounds on the specific discrepancies used in each chapter. These bounds are in general obtained by refining known results in an unweighted setting to the specific weights chosen in each chapter.

- Next, we prove the existence of lattice rules having low bounds on the weighted discrepancy. The existence results are proved by using an averaging argument.

- With the exception of Chapter 4, we then construct lattice rules extensible in dimension by using the component-by-component technique and prove that lattice rules constructed by using this technique satisfy bounds for the weighted discrepancy that have the same order of magnitude as established by the existence results.

- Then we establish tractability and/or strong tractability results by imposing further conditions over the weights. When these additional conditions lead to bounds on the weighted discrepancy that are independent of the dimension, then we ensure strong tractability.

- Attention is also given to the analysis of the computational costs incurred by the construction of lattice rules.

For integrals over the unit cube, much of the earlier work was done by employing a L_2 weighted discrepancy as a criterion of goodness (see for instance [9], [35], [36], [37], or [52]). In the mentioned papers, the integrand was assumed to belong to certain reproducing kernel Hilbert spaces such as weighted Korobov spaces of periodic functions or weighted Sobolev spaces. Often in these spaces it was required that the integrand has square integrable mixed first derivatives. From the bound given by (1.13), we see that the integrand has the weaker requirement of integrable mixed first derivatives. In general terms, the approach used in Chapters 2–5 has the following significant advantages:

- The weighted star discrepancy from (1.13) can be viewed as a L_∞ version of the L_2 discrepancy. For such a version, results are in general much

harder to obtain than for corresponding L_2 versions of the discrepancy. However, in a product weighted setting, once we obtain results for the L_∞ weighted star discrepancy, subsequent results for the L_p weighted discrepancy can be deduced for any $p \geq 1$ (as it is the case for the settings used in Chapters 3 and 5).

- There is no need for a periodicity assumption for the integrand.
- The integrand is of lesser smoothness than usual integrands in the reproducing kernel Hilbert spaces mentioned earlier.

In Chapter 2, we construct rank-1 lattice rules of the form (1.5) with a prime number of points and under the assumption that the weights are general. As a measure of goodness, we use the weighted star discrepancy arising from (1.13) and mentioned in Section 1.2. We construct the generating vector of these lattice rules such that the corresponding weighted star discrepancy is small. We also give special attention to some particular classes of weights and analyse in detail the computational costs incurred by the construction. The material in this chapter is based on the coauthored paper [48]. New contributions in this chapter are given by Lemma 2.4 (due to Stephen Joe), Lemma 2.5, the existence result of Theorem 2.6 followed by the Corollaries 2.7 and 2.8, as well as the construction result (and probably the central result of this chapter) of Theorem 2.11 and Corollaries 2.12, 2.13, 2.14 and 2.15. Also new is the strong tractability result of Theorem 2.16, while Section 2.7 represents an extension of the computational costs analysed in papers such as [6], [9] and [44] adapted to the specific set of hypotheses used in this chapter.

In Chapter 3, we consider intermediate-rank lattice rules of the form (1.7), where we also assume that n is prime, but the weights have a product form (see (1.12)). As in Chapter 2, the generating vector of these lattice rules will also be constructed using the CBC technique. The results of this chapter are based on the coauthored paper [49]. New results are the existence results of Theorem 3.2 and Corollary 3.3 and the construction results of Theorem 3.5

and Corollary 3.6. Known results are extended by Lemma 3.1 and Theorem 3.4 as also mentioned within this chapter. The computational costs analysed in Section 3.5 are based on the results from Appendix A, which at their turn are an extension of the results from [31].

Chapter 4 deals with the lattice rules considered in the previous two chapters, that is, rank-1 lattice rules with general weights and intermediate-rank lattice rules with product weights, but under the assumption that the generating vector is of the Korobov form (1.8). We prove that Korobov-type lattice rules having a low weighted star discrepancy do exist and thus, the results in this chapter will refine the results obtained in Chapters 2 and 3. We also remark that the results from Chapter 4 are new and have not appeared anywhere else in the specialised literature under the assumptions used within this chapter. Original contributions are given by Theorem 4.2 and Corollaries 4.3, 4.4 and 4.5, as well as the results from Theorems 4.6, 4.7 and 4.8.

In many research papers the number of lattice points n was assumed to be prime. This assumption presents some advantages in the sense that the whole analysis is significantly simplified. Since there aren't too many known results for the non-prime case in the specialised literature, in Chapter 5 we contribute to filling such a gap. We consider rank-1 lattice rules having a non-prime number of points with the weights of a product form. By using quite laborious number theory techniques and results, we prove that we can construct generating vectors for these lattice rules having a low weighted star discrepancy. In some sense, this chapter extends the results from [29] to the non-prime case. The material in this chapter is based on the coauthored paper [50]. New results arising from this chapter are stated and proved in Theorems 5.1 and 5.4, Corollaries 5.2 and 5.5 and Lemma 5.3.

Chapters 6 and 7 deal with weighted integrals of the form (1.4) over Euclidean space. The fact that the domain is unbounded raises additional difficulties. First of all, it is not easy to establish a suitable criterion of goodness to construct quadrature points suitable for the approximation of such integrals.

One such criterion based on the "sphere packing density" (some details are given in Chapter 6) was proposed in [54] or [51, Chapter 9.3]. However this criterion is difficult to use due to a lack of practical algorithms. Instead, we propose in Chapter 6 a criterion based on a worst-case error in reproducing kernel Hilbert spaces with the kernel involving the Fourier transform of functions. It is common to transform integrands over unbounded regions to integrals over the unit cube and then employ the techniques used over the unit cube. However it may be possible that the transformed integrand is unbounded near the boundary and for this reason, we use shifted lattice rules of the form (1.6) to deal with such integrands. By using a product weighted setting, we prove that good shifted lattice rules suitable for these integrands can be constructed using a CBC technique. Under a product weighted assumption, similar results were previously established in [38] and [62]. We also test the merit of the lattice rules constructed in this chapter by performing numerical experiments. These numerical experiments suggest that in practice, we may achieve a better convergence than the theoretical $O(n^{-1/2})$. We also remark that a significant part of this chapter consists of new results, especially in Sections 6.5 and 6.6. Original contributions are the results from Theorems 6.6, 6.7 and Corollary 6.8 as well as the numerical experiments of Section 6.6. Theorems 6.4, 6.5 and 6.9 are rather extensions of known results. We should also mention that the results from Appendix B are also new and technically speaking, should have been inserted in Chapter 6. However, because the arguments of Appendix B are based on some laborious calculations with univariate functions and we feel that these results would have disturbed the natural flow of ideas from Chapter 6, we have preferred to write an Appendix containing these results.

In Chapter 7, we also consider shifted lattice rules of the form (1.6) but in a general weighted setting and by employing a "generalised weighted star discrepancy" as a criterion of goodness. In such a setting there aren't any explicit constructions to date for integrals over $\mathbb{R}^d$. The measure of discrepancy considered in this chapter corresponds to the weighted star discrepancy over

the unit cube used in Chapter 2. We will prove that for such a setting, we can construct shifted lattice rules that achieve the optimal convergence rate. This convergence rate has the same order of magnitude as the rate of convergence obtained for integrals over the unit cube. The results in Chapter 7 are based on the paper [47] and original contributions consist of the existence result of Theorem 7.1 followed by Corollaries 7.2 and 7.3, as well as the construction results stated and proved by Theorem 7.4 and Corollary 7.5.

Some of the achievements provided by the results from Chapters 6 and 7 could be briefly summarised as follows:

- Allow the approximation of integrands over unbounded regions in reproducing kernel Hilbert spaces, with the kernel based on the Fourier transforms of functions.

- Allow the construction of shifted lattice rules under both a product weighted and a general weighted assumption.

- An improved convergence order of $O(n^{-1+\delta})$ for any $\delta > 0$ is obtained for the weighted discrepancy from Chapter 7. This convergence is probably optimal for any constructive quasi-Monte Carlo method and is better than the typical $O(n^{-1/2})$ expected from Monte-Carlo methods.

The thesis ends with a brief conclusion indicating the main achievements and pointing out to future research directions.

Chapter 2

Good rank-1 lattice rules based on the general weighted star discrepancy

In this chapter, we study the problem of constructing rank-1 lattice rules having good bounds on the "weighted star discrepancy" with general non-negative weights. In order to show the existence of such good lattice rules, we use an averaging argument and a similar argument is used later to prove that these lattice rules may be obtained using a component-by-component (CBC) construction of the generating vector. Under appropriate conditions on the weights, these lattice rules satisfy strong tractability bounds on the weighted star discrepancy. Particular classes of weights known as "order-dependent" and "finite-order" weights are then considered and we show that the cost of the construction can be very much reduced for these two classes of weights.

2.1 Introduction

Integrals over the d-dimensional unit cube given by

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

may be approximated by rank-1 lattice rules. These are quadrature rules of the form (see also (1.5))

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

where $\boldsymbol{z} \in \mathbb{Z}^d$ is the generating vector whose components are assumed to be relatively prime with n. As mentioned in the first chapter, the braces around a vector indicate that we only take the fractional part of each component of the vector.

Many research papers have been concerned with finding "good" lattice rules. In order to compare the quality of different lattice rules, some criterion needs to be chosen. As mentioned in the previous chapter, a number of criteria are based on the idea of "discrepancy". Such discrepancy measures have been considered in [17], [20], [28], [29] and [41], or in a more general work such as [42]. A classic example is the star discrepancy which appears in the Koksma-Hlawka inequality (see (1.11)). In an unweighted setting, the existence of d-dimensional rank-1 lattice rules having a bound on the star discrepancy of $O\left(n^{-1}(\ln n)^d\right)$ with the implied constant depending only on d, was proved in [41]. A component-by-component (CBC) construction of the generating vector for such rules was given in [28].

In this chapter we are interested in constructing rank-1 lattice rules by using a weighted star discrepancy as a criterion of goodness. In [29] it was shown that lattice rules with good bounds on the weighted star discrepancy do exist and can be obtained by using a CBC construction of $\boldsymbol{z}$ in the situation when n is prime and the weights are of a "product" form (see (1.12)). In Sections 2.3 and 2.4 we extend these results to the general situation where the weights do not necessarily have this product form. Such general weights have been first considered in [9], where it was shown that good lattice rules can be obtained for integrands belonging to weighted Korobov spaces. In these spaces the integrands were assumed to be periodic. For the general weighted star discrepancy considered here, the functions belonging to the associated

function spaces have no such periodicity assumption.

In [21] it is shown that weighted integrals over possibly unbounded domains may be approximated by suitably transforming points in $[0,1]^d$. As we shall explain in Section 2.2, the CBC construction presented here will lead to lattice rules that are appropriate for such weighted integrals. Further details on the construction of lattices for integrals over unbounded regions will be given in Chapters 6 and 7. In Chapter 7, we will construct shifted rank-1 lattice rules (see (1.6)) for integrals over Euclidean space under the same assumptions on the weights as in the present chapter.

There are some applications in which it is the low dimensional projections that are the most important (for instance the ANOVA decomposition mentioned in Chapter 1). In such cases, it is useful to introduce general weights that allow us to model the relative importance of each group of variables. As indicated in [9], weights which are "order-dependent" and/or "finite-order" often provide reasonable assumptions which also present the advantage that the complexity of the CBC construction is drastically reduced. The definitions of these particular classes of weights and the analysis of their computational costs for the CBC construction are given in Sections 2.5 and 2.7.

2.2 General weighted star discrepancy

Let us denote by $\mathfrak{u}$ an arbitrary non-empty subset of $\mathcal{D} = \{1, 2, \ldots, d\}$ and let us mention that for the rest of the thesis, any subset of $\mathcal{D}$ will be considered as being non-empty unless otherwise indicated. Recall that for the vector $\boldsymbol{x} \in [0,1]^d$, $\boldsymbol{x}_\mathfrak{u}$ denotes the vector from $[0,1]^{|\mathfrak{u}|}$ containing the components of $\boldsymbol{x}$ whose indices belong to $\mathfrak{u}$, while by $(\boldsymbol{x}_\mathfrak{u}, \mathbf{1})$ we mean the vector from $[0,1]^d$ whose j-th component is x_j if $j \in \mathfrak{u}$ and 1 if $j \notin \mathfrak{u}$. If P_n denotes the set of quadrature points, then Zaremba's identity (see for instance [57] or [64]) yields:

$$Q_{n,d}(f) - I_d(f) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} (-1)^{|\mathfrak{u}|} \int_{[0,1]^{|\mathfrak{u}|}} \mathrm{discr}((\boldsymbol{x}_\mathfrak{u}, \mathbf{1}), P_n) \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_\mathfrak{u}} f((\boldsymbol{x}_\mathfrak{u}, \mathbf{1}))\, \mathrm{d}\boldsymbol{x}_\mathfrak{u}. \quad (2.1)$$

We recall that the local star discrepancy $\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1})$ is as introduced by Definition 1.4. As an aside, we mention that Zaremba's identity actually represents an extension to the multidimensional case of the formula of integration by parts of Riemann-Stieltjes integrals.

Now let us introduce a set of non-negative weights $\{\boldsymbol{\gamma}_{\mathfrak{u}}\}_{\mathfrak{u}\subseteq\mathcal{D}}$ and consider $\boldsymbol{\gamma}_{\mathfrak{u}}$ as the weight associated with the non-empty set $\mathfrak{u}$. We also assume that the weights are independent of the dimension d. Using (2.1) we see that we can write

$$Q_{n,d}(f) - I_d(f) = \sum_{\mathfrak{u}\subseteq\mathcal{D}} (-1)^{|\mathfrak{u}|} \boldsymbol{\gamma}_{\mathfrak{u}} \int_{[0,1]^{|\mathfrak{u}|}} \mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n) \boldsymbol{\gamma}_{\mathfrak{u}}^{-1} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_{\mathfrak{u}}} f((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}))\, \mathrm{d}\boldsymbol{x}_{\mathfrak{u}}.$$

Applying Hölder's inequality for integrals and sums, we obtain the inequality (1.13) mentioned in Chapter 1, that is

$$\begin{aligned} |Q_{n,d}(f) - I_d(f)| \;\leq\; & \left(\max_{\mathfrak{u}\subseteq\mathcal{D}} \sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} \boldsymbol{\gamma}_{\mathfrak{u}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)| \right) \\ & \times \left(\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_{\mathfrak{u}}} f((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1})) \right| \mathrm{d}\boldsymbol{x}_{\mathfrak{u}} \right). \end{aligned}$$

Thus the weighted star discrepancy $D^*_{n,\boldsymbol{\gamma}}$ of the point set P_n may be defined by

$$D^*_{n,\boldsymbol{\gamma}}(P_n) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)|\,. \tag{2.2}$$

As our interest is in rank-1 lattice rules, from now on we shall assume that P_n is the point set $\{\{k\boldsymbol{z}/n\},\ 0 \leq k \leq n-1\}$. Then we can denote $D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) := D^*_{n,\boldsymbol{\gamma}}(P_n)$.

Let's remark that some of these formulae make sense only for strictly positive weights. If there are some sets $\mathfrak{u} \subseteq \mathcal{D}$ for which $\boldsymbol{\gamma}_{\mathfrak{u}} = 0$, then we adopt the convention that $0 \cdot \infty = 0$ (the same convention has been used in [9]).

As mentioned earlier, there are applications for which the lower dimensional projections are the most important. This suggests that the weight associated with a set should not be bigger than the weights associated with any of its subsets. So we shall make the assumption that for any non-empty subset $\mathfrak{u} \subseteq \mathcal{D}$, we have

$$\boldsymbol{\gamma}_{\mathfrak{u}} \leq \boldsymbol{\gamma}_{\mathfrak{g}} \quad \text{for any} \quad \emptyset \neq \mathfrak{g} \subseteq \mathfrak{u}. \tag{2.3}$$

The next section presents bounds for the general weighted star discrepancy (2.2). This will allow us to prove the existence of good rank-1 lattice rules in the sense of having low bounds on the weighted star discrepancy, while in Section 2.4 we present a CBC construction of the generating vector $\boldsymbol{z}$ of these lattice rules.

2.3 Bounds on the general weighted star discrepancy

We start this section by recalling further general results from the theory of lattice rules (see [42] and [51] for more details).

Definition 2.1 *If L is a lattice in $\mathbb{R}^d$, then its dual lattice is defined by*

$$L^\perp := \{\boldsymbol{h} \in \mathbb{R}^d : \boldsymbol{h} \cdot \boldsymbol{x} \in \mathbb{Z}, \forall \boldsymbol{x} \in L\},$$

where $\cdot$ denotes the usual inner product of vectors.

If L is an integration lattice (see Definition 1.2), then its dual is as given by Definition 2.1 but consisting only of those $\boldsymbol{h}$ in the dual that belong to $\mathbb{Z}^d$. Since the points of a rank-1 lattice rules are given by $\{\{k\boldsymbol{z}/n\} : 0 \le k \le n-1\}$, then the associated integration lattice has the form (see also [51])

$$L = \{\{k\boldsymbol{z}/n\} + \boldsymbol{y} : 0 \le k \le n-1, \boldsymbol{y} \in \mathbb{Z}^d\}.$$

Now we see that for the condition $\boldsymbol{h} \cdot \boldsymbol{x} \in \mathbb{Z}$ to hold for every $\boldsymbol{x} \in L$, we need $\boldsymbol{h} \cdot \boldsymbol{z}$ to be a multiple of n. Hence for this particular case

$$L^\perp = \{\boldsymbol{h} \in \mathbb{Z}^d : \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \,(\mathrm{mod}\, n)\}. \tag{2.4}$$

Consider now a function g defined on $[0,1]^d$ having the absolutely convergent Fourier series representation

$$g(\boldsymbol{y}) = \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \hat{g}(\boldsymbol{h}) e^{2\pi \mathrm{i} \boldsymbol{h} \cdot \boldsymbol{y}}, \quad \boldsymbol{y} \in [0,1]^d,$$

where the $\hat{g}(\boldsymbol{h})$ are the usual Fourier coefficients given by

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

One of the main results for the subsequent error analysis is based on [51, Theorem 2.8]. For completeness, we present this result next:

Theorem 2.1 *Let $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}$ be the points of a lattice rule and let L be the associated integration lattice. Consider the d-dimensional lattice rule given by*

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

If the function g has an absolutely convergent Fourier series representation, then the quadrature error is given by

$$Q_{n,d}(g) - I_d(g) = \sum_{\boldsymbol{h}\in L^\perp}{}' \hat{g}(\boldsymbol{h}), \tag{2.5}$$

where the $'$ in the sum indicates we omit the $\boldsymbol{h} = \boldsymbol{0}$ term. For rank-1 lattice rules, (2.5) *becomes*

$$Q_{n,d}(g) - I_d(g) = \sum_{\boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \,(\bmod\, n)}{}' \hat{g}(\boldsymbol{h}). \tag{2.6}$$

Proof. The proof of this result is based on [42, Lemma 5.21] or [51, Lemma 2.7]. These results state that if $\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}$ are the points of a lattice rule, then

$$\frac{1}{n} \sum_{k=0}^{n-1} e^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{t}_k} = \begin{cases} 1, & \boldsymbol{h} \in L^\perp, \\ 0, & \boldsymbol{h} \notin L^\perp. \end{cases} \tag{2.7}$$

It will follow that

$$Q_{n,d}(g) = \sum_{\boldsymbol{h}\in\mathbb{Z}^d} \hat{g}(\boldsymbol{h}) Q_{n,d}\left(e^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{t}_k}\right).$$

From $I_d(g) = \hat{g}(\boldsymbol{0})$ and (2.7), the desired result follows. For rank-1 lattice rules, (2.6) follows immediately from (2.4). □

Let us define now

$$E^*_{n,s} := \{\boldsymbol{h} \in \mathbb{Z}^s,\ \boldsymbol{h} \neq \boldsymbol{0} : -n/2 < h_j \leq n/2,\ 1 \leq j \leq s\}, \tag{2.8}$$

for any positive integer s. For a fixed integer m independent of n, let's denote $N = nm$ and consider

$$R_N(\boldsymbol{z}, \mathfrak{u}) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(1 + \sum_{-N/2 < h \leq N/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right) - 1. \tag{2.9}$$

It is easy to see that $R_N(\boldsymbol{z}, \mathfrak{u})$ represents the quadrature error produced by applying the rank-1 lattice rule (1.5) to the integrand

$$g_{\mathfrak{u}}(\boldsymbol{x}) = \prod_{j \in \mathfrak{u}} \left(1 + \sum_{-N/2 < h \leq N/2}{}' \frac{e^{2\pi \mathrm{i} h x_j}}{|h|} \right).$$

This function has the Fourier coefficients given by $\hat{g}_{\mathfrak{u}}(\boldsymbol{h}) = \prod_{j \in \mathfrak{u}} \frac{1}{\max(1, |h_j|)}$, if $\boldsymbol{h} \in E^*_{N,|\mathfrak{u}|}$ and 0 otherwise. Hence, it follows from (2.6) that we may write $R_N(\boldsymbol{z}, \mathfrak{u})$ as

$$R_N(\boldsymbol{z}, \mathfrak{u}) := \sum_{\substack{\boldsymbol{h} \in E^*_{N,|\mathfrak{u}|} \\ \boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}} \equiv 0 \,(\bmod\, n)}} \prod_{j \in \mathfrak{u}} \frac{1}{\max(1, |h_j|)}. \tag{2.10}$$

Let us remark that throughout this chapter, we take $N = n$ in (2.9) and (2.10). An analysis requiring $N \neq n$ will be used later in Chapter 7.

At this stage, we mention that it is very hard to compute the weighted star discrepancy as given by (2.2). Instead, we establish upper bounds on the discrepancy and, in order to obtain such bounds, we make use of some results fully stated and proved by Niederreiter in [42] for the unweighted star discrepancy (see Definition 1.5). Since throughout the thesis we use Niederreiter's results several times, we present them below. The first result is [42, Theorem 3.10], which states the following:

Theorem 2.2 *Let $M \geq 2$ be an integer and $\boldsymbol{y}_0, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_{N-1} \subseteq \mathbb{Z}^s$. If P_N is the set consisting of the fractional parts of $M^{-1}\boldsymbol{y}_k$ for all $0 \leq k \leq N-1$, then*

$$D^*(P_N) \leq 1 - \left(1 - \frac{1}{M}\right)^s + \sum_{\boldsymbol{h} \in E^*_{M,s}} \frac{1}{r(\boldsymbol{h}, M)} \left| \frac{1}{N} \sum_{k=0}^{N-1} e^{2\pi \mathrm{i} \boldsymbol{h} \cdot \boldsymbol{y}_k / M} \right|,$$

where $D^*(P_N)$ is the unweighted star discrepancy introduced by Definition 1.5, while $r(\boldsymbol{h}, M) = \prod_{j=1}^{s} r(h_j, M)$ with

$$r(h, M) = \begin{cases} M \sin \frac{\pi |h|}{M}, & \text{if } h \neq 0 \\ 1, & \text{otherwise.} \end{cases}$$

An almost straightforward consequence of this result is [42, Theorem 5.6], which follows from $\sin\ \pi t \geq 2t$ for any $0 \leq t \leq \frac{1}{2}$ and by taking $M = N = n$ in Theorem 2.2. This result is given next.

Theorem 2.3 *If P_n is the point set of a rank-1 lattice rule with $n \geq 2$ distinct points and generating vector $\boldsymbol{z}$, then*

$$D^*(P_n) \leq 1 - \left(1 - \frac{1}{n}\right)^s + \frac{1}{2} \sum_{\substack{\boldsymbol{h} \in E^*_{n,s} \\ \boldsymbol{h}\cdot\boldsymbol{z} \equiv 0 \,(\bmod\ n)}} \prod_{j=1}^{s} \frac{1}{\max(1, |h_j|)}.$$

Using now Theorem 2.3, we obtain

$$\sup_{\boldsymbol{x}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)| \leq 1 - (1 - 1/n)^{|\mathfrak{u}|} + \frac{R_n(\boldsymbol{z}, \mathfrak{u})}{2}, \tag{2.11}$$

where $R_n(\boldsymbol{z}, \mathfrak{u})$ is given by (2.10) with $N = n$. Assuming that $\gcd(z_j, n) = 1$ for $1 \leq j \leq d$, then $\boldsymbol{z}_{\mathfrak{u}}$ is the generating vector for a $|\mathfrak{u}|$-dimensional lattice rule having n distinct points. Recalling that the general weighted star discrepancy defined by (2.2) was also denoted by $D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z})$, we see from (2.11) that we obtain the following inequality:

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \max_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1 - (1 - 1/n)^{|\mathfrak{u}|} + \frac{R_n(\boldsymbol{z}, \mathfrak{u})}{2}\right). \tag{2.12}$$

As an aside, let us remark that the bound in (2.11) also holds for the extreme discrepancy of [42]. This extreme discrepancy is based on the local discrepancy

$$\mathrm{discr}(\boldsymbol{w}, \boldsymbol{x}, P_n) := \frac{|[\boldsymbol{w}, \boldsymbol{x}) \cap P_n|}{n} - \prod_{j=1}^{d} (x_j - w_j),$$

where $0 \leq w_j \leq x_j \leq 1$, $1 \leq j \leq d$. The local star discrepancy of (1.9) is the special case when $w_j = 0$. In [21] and [22] it is shown that it is appropriate to approximate weighted integrals of the form (1.4) over possibly unbounded domains by suitably transforming points from $[0, 1]^d$ to $\mathbb{R}^d$ (such a transformation will be presented in Chapter 6). These points in the unit cube have what is termed a "low weighted L_∞ unanchored discrepancy", which is nothing but the weighted version of the extreme discrepancy of [42]. It follows that the CBC construction presented here will produce lattice rules that also have

a low weighted L_∞ unanchored discrepancy. So such lattice rules are appropriate for weighted integrals over unbounded domains. Further details and a construction of shifted lattice rules for integrals over Euclidean space will be given in Chapters 6 and 7.

Bernoulli's inequality or a simple direct calculation yields

$$(1-1/n)^{|\mathfrak{u}|} \ge 1 - \frac{|\mathfrak{u}|}{n} \quad \text{and so} \quad 1-(1-1/n)^{|\mathfrak{u}|} \le \frac{|\mathfrak{u}|}{n}.$$

This then leads to

$$\max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1-(1-1/n)^{|\mathfrak{u}|}\right) \le \frac{1}{n} \max_{\mathfrak{u}\subseteq\mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}}. \tag{2.13}$$

Now by defining

$$C_k(z) := \sum_{-N/2<h\le N/2}{}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|}, \quad 0 \le k \le n-1,$$

and using the expansion

$$\prod_{j\in\mathfrak{u}} (1+a_j) = 1 + \sum_{\mathfrak{g}\subseteq\mathfrak{u}} \prod_{j\in\mathfrak{g}} a_j, \tag{2.14}$$

we have from (2.9) that

$$\begin{aligned} R_N(\boldsymbol{z},\mathfrak{u}) &= \frac{1}{n}\sum_{k=0}^{n-1} \prod_{j\in\mathfrak{u}} [1+C_k(z_j)] - 1 = \frac{1}{n}\sum_{k=0}^{n-1} \sum_{\mathfrak{g}\subseteq\mathfrak{u}} \prod_{j\in\mathfrak{g}} C_k(z_j) \\ &= \sum_{\mathfrak{g}\subseteq\mathfrak{u}} \frac{1}{n}\sum_{k=0}^{n-1} \prod_{j\in\mathfrak{g}} C_k(z_j) = \sum_{\mathfrak{g}\subseteq\mathfrak{u}} \widetilde{R}_N(\boldsymbol{z},\mathfrak{g}), \end{aligned}$$

where

$$\widetilde{R}_N(\boldsymbol{z},\mathfrak{g}) := \frac{1}{n}\sum_{k=0}^{n-1} \prod_{j\in\mathfrak{g}} \left(\sum_{-N/2<h\le N/2}{}' \frac{e^{2\pi \mathrm{i} hkz_j/n}}{|h|} \right). \tag{2.15}$$

For later use, we note that Theorem 2.1 and the arguments that lead to (2.10) show that with

$$\widetilde{E}^*_{n,s} := \{\boldsymbol{h}\in\mathbb{Z}^s : -n/2 < h_j \le n/2,\ h_j \ne 0,\ 1\le j\le s\}, \tag{2.16}$$

we may write $\widetilde{R}_N(\boldsymbol{z},\mathfrak{g})$ as

$$\widetilde{R}_N(\boldsymbol{z},\mathfrak{g}) = \sum_{\substack{\boldsymbol{h}\in\widetilde{E}^*_{N,|\mathfrak{g}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{g}}\equiv 0 \,(\bmod\ n)}} \prod_{j\in\mathfrak{g}} \frac{1}{|h_j|} \ge 0. \tag{2.17}$$

We see now that for any $\mathfrak{u} \subseteq \mathcal{D}$, we can write

$$\boldsymbol{\gamma}_{\mathfrak{u}} R_N(\boldsymbol{z}, \mathfrak{u}) = \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{\mathfrak{g} \subseteq \mathfrak{u}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{g}).$$

Under the assumption given by (2.3), we obtain

$$\boldsymbol{\gamma}_{\mathfrak{u}} R_N(\boldsymbol{z}, \mathfrak{u}) \leq \sum_{\mathfrak{g} \subseteq \mathfrak{u}} \boldsymbol{\gamma}_{\mathfrak{g}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{g}) \leq \sum_{\mathfrak{g} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{g}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{g}).$$

As a consequence, we then conclude that

$$\max_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} R_N(\boldsymbol{z}, \mathfrak{u}) \leq \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}). \tag{2.18}$$

For $N = n$, the inequality (2.18) combined with (2.12) and (2.13) yields the following result:

Lemma 2.4 *If the weights $\boldsymbol{\gamma}_{\mathfrak{u}}$ satisfy (2.3) for any $\mathfrak{u} \subseteq \mathcal{D}$, then*

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{1}{n} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2} e^2_{n,d}(\boldsymbol{z}),$$

where

$$e^2_{n,d}(\boldsymbol{z}) := \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}). \tag{2.19}$$

Let us mention that a similar result with $N \neq n$ will be deduced later in Chapter 7.

Let us also remark that throughout the thesis, the quantity $e^2_{n,d}(\boldsymbol{z})$ will have several different expressions. Since these quantities have related meanings, we prefer to use the same notation for consistency purposes.

Lemma 2.4 shows that we can analyse the weighted star discrepancy by considering the quantity $e^2_{n,d}(\boldsymbol{z})$. Let us also remark that in other settings this quantity represents a square worst-case error (as in Chapter 6 or [9]). This justifies the use of the exponent in the notation of $e^2_{n,d}(\boldsymbol{z})$.

For the rest of the chapter, we shall assume that n is prime. Because we only consider the fractional part of each component of $k\boldsymbol{z}/n$, we see that we may take each component of the generating vector $\boldsymbol{z}$ as belonging to the set $\mathcal{Z}_n = \{1, 2, \ldots, n-1\}$. We can obtain bounds on $e^2_{n,d}(\boldsymbol{z})$ for the case in which

n is prime by obtaining an expression for a certain mean value of $e_{n,d}^2(\boldsymbol{z})$. The mean is taken over all integer vectors $\boldsymbol{z} \in \mathcal{Z}_n^d$ and is defined by

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

Before finding an expression for the mean, we need the following auxiliary result (this will also be useful in Chapter 3 and Chapter 7):

Lemma 2.5 *Let n be prime and m be a fixed integer with $N = nm$. If we denote*

$$T_N(k) = \frac{1}{n-1} \sum_{z=1}^{n-1} {\sum_{-\frac{N}{2} < h \le \frac{N}{2}}}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|}, \tag{2.20}$$

where $1 \le k \le n-1$, then

$$T_N(k) = \frac{S_m - S_N}{n-1}, \tag{2.21}$$

where

$$S_n := {\sum_{-n/2 < h \le n/2}}' \frac{1}{|h|}.$$

If $N = n$, then

$$T_n(k) = -\frac{S_n}{n-1}.$$

Proof. By separating out the terms for which $h \equiv 0 \,(\mathrm{mod}\, n)$ and replacing h with nq for such terms, we obtain

$$\begin{aligned} T_N(k) &= \frac{1}{n-1} \left(\sum_{z=1}^{n-1} {\sum_{\substack{-\frac{N}{2} < h \le \frac{N}{2} \\ h \equiv 0 \,(\mathrm{mod}\, n)}}}' \frac{1}{|h|} + \sum_{z=1}^{n-1} {\sum_{\substack{-\frac{N}{2} < h \le \frac{N}{2} \\ h \not\equiv 0 \,(\mathrm{mod}\, n)}}}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|} \right) \\ &= \frac{1}{n-1} \left(\sum_{z=1}^{n-1} {\sum_{-\frac{N}{2} < nq \le \frac{N}{2}}}' \frac{1}{n|q|} + {\sum_{\substack{-\frac{N}{2} < h \le \frac{N}{2} \\ h \not\equiv 0 \,(\mathrm{mod}\, n)}}}' \frac{1}{|h|} \sum_{z=1}^{n-1} \left(e^{2\pi \mathrm{i} hk/n} \right)^z \right). \end{aligned}$$

Since n is prime and in the second sum $hk \not\equiv 0 \,(\mathrm{mod}\, n)$, it is easy to check that

$$\sum_{z=1}^{n-1} \left(e^{2\pi \mathrm{i} hk/n} \right)^z = -1. \tag{2.22}$$

Indeed, we can write

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

Replacing in the expression for $T_N(k)$ we obtain:

$$T_N(k) = \frac{1}{n}S_{N/n} - \frac{1}{n-1}\sum_{\substack{-\frac{N}{2}<h\le\frac{N}{2}\\ h\not\equiv 0 \,(\bmod\, n)}}{}' \frac{1}{|h|}.$$

The last term of the sum may be written as:

$$\begin{aligned}\sum_{\substack{-\frac{N}{2}<h\le\frac{N}{2}\\ h\not\equiv 0 \,(\bmod\, n)}}{}' \frac{1}{|h|} &= \sum_{-\frac{N}{2}<h\le\frac{N}{2}}{}' \frac{1}{|h|} - \sum_{-\frac{N}{2}<nq\le\frac{N}{2}}{}' \frac{1}{n|q|}\\ &= S_N - \frac{1}{n}\sum_{-\frac{N}{2n}<q\le\frac{N}{2n}}{}' \frac{1}{|q|} = S_N - \frac{1}{n}S_{N/n}.\end{aligned}$$

Thus we obtain:

$$T_N(k) = \frac{S_{N/n}}{n} - \frac{1}{n-1}\left(S_N - \frac{1}{n}S_{N/n}\right) = \frac{S_{N/n}-S_N}{n-1} = \frac{S_m - S_N}{n-1}.$$

In the particular case when $N = n$, then $S_m = S_1 = 0$, and the second part follows immediately. □

An expression for the mean is given in the next theorem:

Theorem 2.6 *Let n be prime. Then*

$$M_{n,d,\boldsymbol{\gamma}} = \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}S_n^{|\mathfrak{u}|} + \frac{n-1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\left(-\frac{S_n}{n-1}\right)^{|\mathfrak{u}|},$$

where S_n is as defined in Lemma 2.5.

Proof. From the definition of the mean, (2.15) and (2.19), we have

$$M_{n,d,\boldsymbol{\gamma}} = \frac{1}{(n-1)^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\left(\frac{1}{n}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}\left(\sum_{-n/2<h\le n/2}{}' \frac{e^{2\pi ihkz_j/n}}{|h|}\right)\right).$$

By separating out the $k=0$ term, we obtain

$$M_{n,d,\boldsymbol{\gamma}} = \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}S_n^{|\mathfrak{u}|} + T_{n,d,\boldsymbol{\gamma}}, \tag{2.23}$$

where

$$\begin{aligned} T_{n,d,\boldsymbol{\gamma}} &= \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\frac{1}{n} \sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} \right) \right) \\ &= \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u}} \left(\frac{1}{n-1} \sum_{z_j=1}^{n-1} \sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} \right) \right). \end{aligned}$$

It follows from Lemma 2.5 that

$$\frac{1}{n-1} \sum_{z_j=1}^{n-1} \sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} = T_n(k) = -\frac{S_n}{n-1},$$

for any $1 \le k \le n-1$, which leads to

$$T_{n,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{k=1}^{n-1} \left(-\frac{S_n}{n-1} \right)^{|\mathfrak{u}|} = \frac{n-1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(-\frac{S_n}{n-1} \right)^{|\mathfrak{u}|}.$$

Replacing now the last term in (2.23) with this expression, we obtain the desired result. □

In the case $d = 1$, it is easy to verify by replacing in the expression for the mean that $M_{n,1,\{\gamma_{\{1\}}\}} = 0$. This is to be expected since whenever $|\mathfrak{g}| = 1$, by making use of (2.15) and Lemma 2.5, we obtain

$$\widetilde{R}_n(z, \mathfrak{g}) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z/n}}{|h|} = \frac{S_n}{n} + \frac{1}{n}(-S_n) = 0.$$

Corollary 2.7 *Let n be prime. Then there exists a generating vector $\boldsymbol{z}$ such that*

$$e_{n,d}^2(\boldsymbol{z}) \le M_{n,d,\boldsymbol{\gamma}} \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}.$$

Proof. The first inequality is obvious. The proof of the second inequality is based on the proof of the second assertion in [9, Theorem 1]. We can write the expression for $M_{n,d,\boldsymbol{\gamma}}$ as

$$M_{n,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} (1 + W_n(\mathfrak{u})),$$

where

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

If $|\mathfrak{u}|$ is odd, then $-1 \leq W_n(\mathfrak{u}) \leq 0$. On the other hand, if $|\mathfrak{u}|$ is even, then $|\mathfrak{u}| \geq 2$ and

$$W_n(\mathfrak{u}) \leq (n-1)\left(\frac{1}{n-1}\right)^2 = \frac{1}{n-1}.$$

So for $|\mathfrak{u}|$ either odd or even, we have $W_n(\mathfrak{u}) \leq 1/(n-1)$ and hence

$$M_{n,d,\boldsymbol{\gamma}} \leq \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}\left(1+\frac{1}{n-1}\right) = \frac{1}{n-1}\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|},$$

which completes the proof. □

This corollary and Lemma 2.4 then lead to the following result:

Corollary 2.8 *Suppose the weights satisfy* (2.3) *and suppose that n is prime. Then there exists a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that the general weighted star discrepancy satisfies the bound*

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{1}{n}\max_{\mathfrak{u}\subseteq\mathcal{D}} |\mathfrak{u}|\boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2(n-1)}\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}.$$

Before further analysing the bound for the weighted star discrepancy, we need a result that was fully stated and proved in [41, Lemmas 1 and 2] and will be useful several times throughout the thesis. This result is:

Lemma 2.9 *If $m \geq 2$ is an integer and*

$$S_m = \sum_{-m/2<h\leq m/2}{}' \frac{1}{|h|},$$

then

$$S_m = 2\ln m + 2\omega - \ln 4 + \varepsilon(m),$$

where ω is the Euler-Mascheroni constant defined by $\omega = \lim_{m\to\infty}\left(\sum_{k=1}^{m}\frac{1}{k} - \ln m\right)$, while $-4/m^2 < \varepsilon(m) \leq 0$ if m is even and $-3/m^2 < \varepsilon(m) < 1/m^2$ if m is odd.

A straightforward consequence of this lemma is:

Corollary 2.10 *If $m \geq 1$ is an integer, then*

$$S_m \leq 2\ln m. \tag{2.24}$$

Proof. An approximate value for $2\omega - \ln 4$ is -0.2319. So for any $m \geq 3$, it will follow from Lemma 2.9 that $S_m \leq 2 \ln m$. A direct calculation then shows that this inequality also holds for $m = 1$ and $m = 2$. $\square$

From Corollary 2.8 and Corollary 2.10, we conclude that for any prime n, there exists a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that the general weighted star discrepancy satisfies the following bound:

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{1}{n} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2(n-1)} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} (2 \ln n)^{|\mathfrak{u}|}. \tag{2.25}$$

Let $\Gamma = \max\limits_{1 \leq j \leq d} \boldsymbol{\gamma}_{\{j\}}$. Since $\boldsymbol{\gamma}_{\mathfrak{u}} \leq \Gamma$ for all $\mathfrak{u} \subseteq \mathcal{D}$ (because of (2.3)) then we have $\max\limits_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} \leq \Gamma d$. Hence from (2.25) we obtain

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{\Gamma d}{n} + \frac{1}{2(n-1)} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} (2 \ln n)^{|\mathfrak{u}|}.$$

Moreover, we have

$$\sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} (2 \ln n)^{|\mathfrak{u}|} \leq \Gamma \sum_{\mathfrak{u} \subseteq \mathcal{D}} (2 \ln n)^{|\mathfrak{u}|} = \Gamma \sum_{j=1}^{d} \binom{d}{j} (2 \ln n)^j \leq \Gamma (1 + 2 \ln n)^d.$$

This yields

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = O\left(n^{-1} (\ln n)^d\right), \tag{2.26}$$

with the implied constant depending only on d and Γ.

In the situation when all the weights are equal to 1, then

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = \max_{\mathfrak{u} \subseteq \mathcal{D}} \sup_{\boldsymbol{x}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)| = \sup_{\boldsymbol{x} \in [0,1]^d} |\mathrm{discr}(\boldsymbol{x}, P_n)|$$

is the unweighted star discrepancy defined in (1.10). For this quantity, the rate of $O\left(n^{-1} (\ln n)^d\right)$ is essentially the best possible (see [34], [39] or [42]). In fact from [39], it follows that the best lower bound for $e^2_{n,d}(\boldsymbol{z})$ as given by (2.19) is $O\left(n^{-1} (\ln n)^d\right)$. Hence the bound for the weighted star discrepancy given in Corollary 2.8 is essentially the best possible and so, we consider such a bound to be "good".

2.4 Component-by-component construction of the generating vector

Because the total number of vectors $\boldsymbol{z} \in \mathcal{Z}_n^d$ is $(n-1)^d$, it is unrealistic to search over all these vectors to find a good one when d and n are large. In this section we propose a cheaper construction of the generating vector, namely the CBC construction. We recall from Section 1.4 that the CBC construction means the generating vector is found one component at a time. When we add a new component to the generating vector, the existing components will stay unchanged. Such a CBC construction was first used in [55] and then successfully employed in several other research papers including [9], [28], [29], [35], [36], [37], [38], [52], [62] as well as in [48], [49], [50] and [47]. The algorithm is given below:

Component-by-component algorithm

1. Set the value for the first component of the vector, say $z_1 = 1$.

2. For $m = 2, 3, \ldots, d$, find $z_m \in \mathcal{Z}_n$ such that $e_{n,m}^2(z_1, \ldots, z_m)$ is minimised. Here

$$e_{n,m}^2(z_1, \ldots, z_m) = \sum_{\mathfrak{u} \subseteq \{1,2,\ldots,m\}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n((z_1, \ldots, z_m), \mathfrak{u}).$$

Our goal is to prove that this algorithm does indeed yield good lattice rules. By good, we mean that the generating vector $\boldsymbol{z}$ found this way satisfies the bound for $e_{n,d}^2(\boldsymbol{z})$ given in Corollary 2.7. The following theorem and corollary justify the use of the CBC algorithm.

Theorem 2.11 *Let n be prime. Suppose there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$e_{n,d}^2(\boldsymbol{z}) \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}. \tag{2.27}$$

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

$$e_{n,d+1}^2(\boldsymbol{z}, z_{d+1}) \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|},$$

where $\mathcal{D}_1 := \mathcal{D} \cup \{d+1\}$. Such a z_{d+1} can be found by minimising $e_{n,d+1}^2(\boldsymbol{z}, z_{d+1})$ over the set $\mathcal{Z}_n$.

Proof. Let us remark first that technically speaking we should use $e^2_{n,d+1}((\boldsymbol{z}, z_{d+1}))$ for $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$, but we prefer not to overload the notation in the arguments that follow. We now have

$$\begin{aligned} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) &= \sum_{\mathfrak{u}\subseteq\mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n((\boldsymbol{z}, z_{d+1}), \mathfrak{u}) \\ &= \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}) + \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n((\boldsymbol{z}, z_{d+1}), \mathfrak{u}). \quad (2.28) \end{aligned}$$

We recall that we defined

$$C_k(z) = \sum_{-n/2<h\le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z/n}}{|h|}, \quad 0 \le k \le n-1.$$

Then clearly $C_0(z) = S_n$. For $\mathfrak{u} \subseteq \mathcal{D}_1$ with $d+1 \in \mathfrak{u}$, we then have

$$\begin{aligned} \widetilde{R}_n((\boldsymbol{z}, z_{d+1}), \mathfrak{u}) &= \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j\in\mathfrak{u}} C_k(z_j) \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \left(\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) \right) C_k(z_{d+1}) \\ &= \frac{S_n^{|\mathfrak{u}|}}{n} + \frac{1}{n} \sum_{k=1}^{n-1} \left(\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) \right) C_k(z_{d+1}), \end{aligned}$$

where the $k=0$ term was separated out. Let us recall that if $|\mathfrak{u}| = 1$, then $\widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}) = 0$, so the contribution to the quantity $e^2_{n,d}(\boldsymbol{z})$ comes only from sets having $|\mathfrak{u}| \ge 2$. By substituting in (2.28), we obtain

$$\begin{aligned} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) &= e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \\ &\quad + \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \frac{\boldsymbol{\gamma}_{\mathfrak{u}}}{n} \sum_{k=1}^{n-1} \left(\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) \right) C_k(z_{d+1}). \end{aligned}$$

Next we average $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over all possible values of $z_{d+1} \in \mathcal{Z}_n$ and consider

$$\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) = \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}).$$

As the dependency of $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ on z_{d+1} is only through the $C_k(z_{d+1})$ factor, we next focus on the quantity

$$T_n(k) = \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} C_k(z_{d+1}).$$

From Lemma 2.5, we have

$$T_n(k) = -\frac{S_n}{n-1}, \quad 1 \le k \le n-1.$$

It follows that

$$\begin{aligned} & \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \\ = \; & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} - \frac{S_n}{n(n-1)} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u} - \{d+1\}} C_k(z_j). \end{aligned}$$

For any $\mathfrak{u} \subseteq \mathcal{D}_1$ with $d+1 \in \mathfrak{u}$ and $|\mathfrak{u}| \ge 2$, we have

$$-\frac{1}{n} \sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u} - \{d+1\}} C_k(z_j) = -\widetilde{R}_n(\boldsymbol{z}, \mathfrak{u} - \{d+1\}) + \frac{S_n^{|\mathfrak{u}|-1}}{n} \le \frac{S_n^{|\mathfrak{u}|-1}}{n},$$

where we have subtracted and added the $k = 0$ term and used the fact that the quantities $\widetilde{R}_n(\boldsymbol{z}, \mathfrak{g})$ are positive (see (2.17)) for any subset $\mathfrak{g} \subseteq \mathcal{D}$. Consequently, we have

$$\begin{aligned} & \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \\ \le \; & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} + \frac{1}{n(n-1)} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \\ = \; & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n-1} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}. \end{aligned}$$

Using the hypothesis, we next obtain

$$\begin{aligned} \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \; & \le \; \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} + \frac{1}{n-1} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D}_1 \\ d+1 \in \mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \\ & = \; \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}. \end{aligned} \tag{2.29}$$

There exists at least one $z_{d+1} \in \mathcal{Z}_n$ such that $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \le \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}))$ and this z_{d+1} may be chosen by minimising $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over the set $\mathcal{Z}_n$. From (2.29), it is clear now that for the chosen z_{d+1}, we have

$$e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|},$$

which is the desired result. □

From this result we can deduce the following:

Corollary 2.12 *Let n be prime. Then for any $1 \leq m \leq d$ we can construct a vector $\boldsymbol{z} \in \mathcal{Z}_n^m$ such that*

$$e_{n,m}^2(z_1, \ldots, z_m) \leq \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \{1,2,\ldots,m\}} \gamma_{\mathfrak{u}} S_n^{|\mathfrak{u}|}.$$

We can set $z_1 = 1$ and for $2 \leq m \leq d$, every z_m can be found by minimising $e_{n,m}^2(z_1, \ldots, z_m)$ over the set $\mathcal{Z}_n$.

Proof. Recall that $\widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}) = 0$ for all subsets $\mathfrak{u} \subseteq \mathcal{D}$ with $|\mathfrak{u}| = 1$. It follows that $e_{n,1}^2(z) = 0$ for any $z \in \mathcal{Z}_n$, so the inequality (2.27) holds for $d = 1$. The result then follows immediately from Theorem 2.11. □

We remark that the approach to the general weighted case used here is slightly different to the approach used in [29] for the product weighted case. If we apply the results obtained here to that case, then the bounds on the weighted star discrepancy are better than those in [29]. However, the approach in [29] has the advantage that it yields bounds on the weighted L_p discrepancy, whereas here we are essentially restricted to the L_∞ case. This limitation essentially occurs because in the expression for (2.15) all the components of $\boldsymbol{h}$ are different from 0, while in [29] or in Chapter 3, we allow $\boldsymbol{h}$ to have up to $d-1$ components equal to 0. More details on the weighted L_p star discrepancy will be given in Section 3.6, in the context of a product weighted setting.

2.5 The CBC construction for special classes of weights

In practical situations the weights may satisfy further assumptions. Special classes of weights are the so-called "order-dependent" and "finite-order" weights, which were mentioned in the first section and first used in [9]. As we shall see in Section 2.7, the computational cost of the CBC construction is

significantly reduced for these particular classes of weights. Order-dependent weights are defined as follows:

Definition 2.2 *Weights are named order-dependent if sets having the same cardinality have equal values of the associated weights.*

Obviously, for order-dependent weights, their dependence on $\mathfrak{u}$ is only through the cardinality of $\mathfrak{u}$. So, it turns that instead of using 2^d-1 weights, we can use just d weights, say $\Gamma_1, \Gamma_2, \ldots, \Gamma_d$, where Γ_ℓ denotes the weight associated with any set containing ℓ elements for $1 \leq \ell \leq d$. For the bound on the weighted star discrepancy given in Lemma 2.4 to hold, it turns from (2.3) that these weights are in non-increasing order, that is, $\Gamma_1 \geq \Gamma_2 \geq \cdots \geq \Gamma_d$.

The next result follows directly from Theorem 2.11, Corollary 2.12 and Corollary 2.10 by taking $\boldsymbol{\gamma}_\mathfrak{u} = \Gamma_\ell$ whenever $|\mathfrak{u}| = \ell$ and noting that the number of subsets of $\mathcal{D}$ with cardinality ℓ is $\binom{d}{\ell}$.

Corollary 2.13 *Let n be prime and suppose the weights are order-dependent. Then a generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that*

$$e_{n,d}^2(\boldsymbol{z}) \leq \frac{1}{n-1} \sum_{\ell=1}^{d} \Gamma_\ell \binom{d}{\ell} S_n^\ell \leq \frac{1}{n-1} \sum_{\ell=1}^{d} \Gamma_\ell \binom{d}{\ell} (2 \ln n)^\ell.$$

Finite-order weights are defined as follows:

Definition 2.3 *Weights are named finite-order if there exists a positive integer q such that $\boldsymbol{\gamma}_\mathfrak{u} = 0$ for all $\mathfrak{u}$ with $|\mathfrak{u}| > q$.*

We shall take q^* to be the smallest integer satisfying this condition. Of course, it makes sense to assume that $q^* < d$, otherwise it will be no different from the situation already discussed. We then obtain the following result:

Corollary 2.14 *Let n be prime and suppose the weights are finite-order. Then a generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that*

$$e_{n,d}^2(\boldsymbol{z}) \leq \frac{1}{n-1} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D} \\ 1 \leq |\mathfrak{u}| \leq q^*}} \boldsymbol{\gamma}_\mathfrak{u} S_n^{|\mathfrak{u}|} \leq \frac{1}{n-1} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D} \\ 1 \leq |\mathfrak{u}| \leq q^*}} \boldsymbol{\gamma}_\mathfrak{u} (2 \ln n)^{|\mathfrak{u}|}.$$

We can combine these two classes of weights to consider the situation when the weights are both order-dependent and finite-order.

Corollary 2.15 *Let n be prime and suppose the weights are both order-dependent and finite-order. Then a generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that*

$$e_{n,d}^2(\boldsymbol{z}) \le \frac{1}{n-1} \sum_{\ell=1}^{q^*} \Gamma_\ell \binom{d}{\ell} S_n^\ell \le \frac{1}{n-1} \sum_{\ell=1}^{q^*} \Gamma_\ell \binom{d}{\ell} (2 \ln n)^\ell.$$

Lattice rules with order-dependent and/or finite-order weights present the advantage that the costs of the CBC construction are significantly reduced. The computational costs of the CBC construction are analysed in Section 2.7.

2.6 Tractability results

Let's remark first that the bound for the weighted star discrepancy obtained in (2.26) is dependent on the dimension d. Obviously, the constant involved will grow with the dimension and this leads to the so-called "curse of dimensionality". As we mentioned in Chapter 1, the curse of dimensionality leads to intractability of the integration problem. However appropriate conditions on the weights do allow us to obtain tractability and strong tractability results and such results will emphasise the real importance of the weights.

Sufficient conditions for tractability and strong tractability in a general weighted setting have been previously established in [9], [20], and [24]. Below, we prove a condition for strong tractability in the context of the assumptions used in this chapter.

Theorem 2.16 *Let us assume that $n \ge 3$ and the weights are such that* (2.3) *is satisfied and*

$$\sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \le C(\boldsymbol{\gamma}, \delta) n^\delta,$$

for some $\delta > 0$, where $C(\boldsymbol{\gamma}, \delta)$ is independent of d and n. Then the CBC algorithm yields a $\boldsymbol{z}$ for which the weighted star discrepancy of the corresponding

lattice rule satisfies the strong tractability error bound

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq 2C(\boldsymbol{\gamma},\delta)n^{-1+\delta}.$$

Proof. From Lemma 2.4, Theorem 2.11 and the hypothesis, we obtain

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{1}{n}\max_{\mathfrak{u}\subseteq\mathcal{D}} |\mathfrak{u}|\boldsymbol{\gamma}_{\mathfrak{u}} + \frac{C(\boldsymbol{\gamma},\delta)n^{\delta}}{2(n-1)}.$$

Since S_n is an increasing function of n and $S_3 = 2$, observe that if $n \geq 3$, then $|\mathfrak{u}| \leq S_n^{|\mathfrak{u}|}$. This leads to

$$\max_{\mathfrak{u}\subseteq\mathcal{D}} |\mathfrak{u}|\boldsymbol{\gamma}_{\mathfrak{u}} \leq \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \leq C(\boldsymbol{\gamma},\delta)n^{\delta}.$$

Consequently, we have

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{C(\boldsymbol{\gamma},\delta)n^{\delta}}{n} + \frac{C(\boldsymbol{\gamma},\delta)n^{\delta}}{2(n-1)} \leq 2C(\boldsymbol{\gamma},\delta)n^{-1+\delta}.$$

Now let us recall from the first chapter (see Definition 1.7) that strong tractability means that the minimal number of function evaluations required to reduce the initial error by a factor of $\varepsilon \in (0,1)$ is bounded by $C\varepsilon^{-p}$ with a constant $C > 0$ independent of d. Hence, the essential idea consists in finding a bound for the weighted star discrepancy that is independent of the dimension. Hence, if we want the condition $D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \varepsilon I_d(f)$ to hold, then we obtain that $n \geq (2C(\boldsymbol{\gamma},\delta))^{\frac{1}{1-\delta}} I_d(f)^{-\frac{1}{1-\delta}} \varepsilon^{-\frac{1}{1-\delta}}$ and so, the minimum number of function values required satisfies

$$n(\varepsilon) \leq \lfloor (2C(\boldsymbol{\gamma},\delta))^{\frac{1}{1-\delta}} I_d(f)^{-\frac{1}{1-\delta}} \varepsilon^{-\frac{1}{1-\delta}} \rfloor + 1.$$

Thus we obtain strong tractability with ε-exponent $1/(1-\delta)$. □

An example of weights $\boldsymbol{\gamma}_{\mathfrak{u}}$ satisfying this strong tractability result is when $\boldsymbol{\gamma}_{\mathfrak{u}}$ are product weights (see (1.12)), and the γ_j satisfy the summability condition $\sum_{j=1}^{\infty} \gamma_j < \infty$. Later in the thesis, namely in Section 3.3, we will prove such a result when we study the tractability problem under a product weighted setting (see Theorem 3.4).

Let us also remark that finite-order weights always imply tractability of the integration problem. In-depth details of such a result are in [56]. Here,

by recalling that $\Gamma = \max_{1\le j\le d} \boldsymbol{\gamma}_{\{j\}}$ and using the condition (2.3), we see from Corollary 2.14 that we can write:

$$e^2_{n,d}(\boldsymbol{z}) \le \frac{\Gamma}{n-1}\sum_{\ell=1}^{q^*}\binom{d}{\ell}S_n^\ell \le \frac{\Gamma}{n-1}\sum_{\ell=1}^{q^*}\binom{d}{\ell}S_n^\ell.$$

Now, we can prove by induction that for $d \ge 2$ and $q^* < d$, we have

$$\sum_{\ell=1}^{q^*}\binom{d}{\ell} \le d^{q^*}. \tag{2.30}$$

Since $S_n = O(\ln n)$ (see Corollary 2.10) and q^* is independent of d, it follows that for any $\delta > 0$, there exist a suitable constant $C > 0$ independent of d but depending on δ and q^* such that $S_n^{q^*} \le Cn^\delta$. This together with (2.30) leads to

$$e^2_{n,d}(\boldsymbol{z}) \le C_1 n^{-1+\delta} d^{q^*},$$

for some constant $C_1 > 0$. This ensures tractability with ε-exponent $1/(1-\delta)$ and d-exponent $q^*/(1-\delta)$ without further conditions on the weights.

2.7 Computational costs of the CBC algorithm

2.7.1 The cost of the CBC algorithm in the general case

In this subsection we analyse the complexity of the CBC algorithm, which was presented in Section 2.4.

In order to analyse the cost of the construction, first recall from (2.15) that $\widetilde{R}_n(\boldsymbol{z},\mathfrak{u})$ is given by

$$\widetilde{R}_n(\boldsymbol{z},\mathfrak{u}) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}} C_k(z_j), \quad \text{where} \quad C_k(z) = \sum_{-n/2<h\le n/2}{}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|}.$$

It is easy to see that the cost of calculating each $\widetilde{R}_n(\boldsymbol{z},\mathfrak{u})$ by using this formula is $O\left(n^2|\mathfrak{u}|\right)$ operations. However, it is shown in Appendix A (see also [29] and [31]) that this cost can be reduced at the expense of extra storage. The idea is based on the fact that $\{kz_j/n\} = \ell/n$ for some ℓ satisfying $0 \le \ell \le n-1$. So to calculate $\widetilde{R}_n(\boldsymbol{z},\mathfrak{u})$, we need the values of

$$\sum_{-n/2<h\le n/2}{}' \frac{e^{2\pi \mathrm{i} h\ell/n}}{|h|},$$

for $0 \le \ell \le n-1$. As shown in [31], these n values may be calculated at a total cost of $O(n)$ operations and then stored. It follows that the number of operations required to calculate each $\widetilde{R}_n(\boldsymbol{z}, \mathfrak{u})$ is of $O(n|\mathfrak{u}|)$ operations at the expense of $O(n)$ extra storage.

Recall that

$$\begin{aligned} e^2_{n,m}(z_1,\ldots,z_m) &= \sum_{\mathfrak{u}\subseteq\{1,2,\ldots,m\}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n((z_1,\ldots,z_m),\mathfrak{u}) \\ &= e^2_{n,m-1}(z_1,\ldots,z_{m-1}) + \sum_{\substack{\mathfrak{u}\subseteq\{1,2,\ldots,m\} \\ m\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n((z_1,\ldots,z_m),\mathfrak{u}) \\ &= e^2_{n,m-1}(z_1,\ldots,z_{m-1}) \\ &\quad + \frac{1}{n} \sum_{\substack{\mathfrak{u}\subseteq\{1,2,\ldots,m\} \\ m\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{k=0}^{n-1} C_k(z_m) \prod_{j\in\mathfrak{u}-\{m\}} C_k(z_j). \end{aligned} \tag{2.31}$$

Now it may be the case that some of the $2^d - 1$ weights are zero. To take into account the computational savings that arise, let τ_m be the number of non-zero weights $\boldsymbol{\gamma}_{\mathfrak{u}}$ for which $\mathfrak{u} \subseteq \{1, 2, \ldots, m\}$ with $m \in \mathfrak{u}$. Then $0 \le \tau_m \le 2^{m-1}$. Also, let τ be the total number of non-zero weights, that is,

$$\tau = \sum_{m=1}^{d} \tau_m \le 2^d - 1.$$

Then to find z_m which minimises $e^2_{n,m}(z_1, \ldots, z_m)$, we need to calculate the last term in (2.31) for each $z_m \in \mathcal{Z}_n$. This requires $O(nm\tau_m)$ operations. Since there are $n-1$ choices for z_m, this means that the cost of adding a new component z_m to the already existing components is $O(n^2 m \tau_m)$ operations for each m. Taking m from 2 to d, we conclude that the total operation count of the CBC algorithm to obtain a d-dimensional $\boldsymbol{z}$ is $O(n^2 d\tau)$.

Let's observe that if all the weights are non-zero, we have a total of $\tau = 2^d - 1$ weights and so the total cost of the construction will be $O(n^2 d 2^d)$. In practice such a cost is unacceptable as 2^d grows very quickly when d increases, but it can be considerably reduced for order-dependent and/or finite-order weights.

2.7.2 The cost of the construction for finite-order weights

Let q^* be the smallest integer for which $\boldsymbol{\gamma}_{\mathfrak{u}} = 0$ whenever $|\mathfrak{u}| > q^*$. In this case, by using (2.30), we see that the total number of non-zero weights is $\tau = \sum_{\ell=1}^{q^*} \binom{d}{\ell} \leq d^{q^*}$.

From the previous subsection, it will follow that the total operation count of the CBC algorithm with finite-order weights is then $O(n^2 d^{q^*+1})$. As pointed out in [9], the cost of the construction is exponential in d, but this is not dangerous as long as q^* is small.

2.7.3 The cost of the construction for order-dependent weights

In this case, because there are at most d distinct weights, the cost of the construction can be significantly reduced by using a similar technique as in [9]. First, let's observe that the quantity $e^2_{n,m}(z_1, z_2, \ldots, z_m)$ can be expanded as

$$\begin{aligned} e^2_{n,m}(z_1, z_2, \ldots, z_m) &= \sum_{\ell=1}^{m} \Gamma_\ell \sum_{\substack{\mathfrak{u} \subseteq \{1,2,\ldots,m\} \\ |\mathfrak{u}|=\ell}} \widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}) \\ &= \sum_{\ell=1}^{m} \Gamma_\ell \sum_{\substack{\mathfrak{u} \subseteq \{1,2,\ldots,m\} \\ |\mathfrak{u}|=\ell}} \left(\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} C_k(z_j) \right) \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\ell=1}^{m} \Gamma_\ell \sigma_k(m, \ell), \end{aligned}$$

where

$$\sigma_k(m, \ell) = \sum_{\substack{\mathfrak{u} \subseteq \{1,2,\ldots,m\} \\ |\mathfrak{u}|=\ell}} \prod_{j \in \mathfrak{u}} C_k(z_j) \quad \text{for} \quad 1 \leq \ell \leq m.$$

Then we can obtain a recursive formula to compute the quantities $\sigma_k(m, \ell)$. Indeed, we have

$$\begin{aligned} \sigma_k(m, \ell) &= \sum_{\substack{\mathfrak{u} \subseteq \{1,2,\ldots,m-1\} \\ |\mathfrak{u}|=\ell}} \prod_{j \in \mathfrak{u}} C_k(z_j) + C_k(z_m) \sum_{\substack{\mathfrak{u} \subseteq \{1,2,\ldots,m-1\} \\ |\mathfrak{u}|=\ell-1}} \prod_{j \in \mathfrak{u}} C_k(z_j) \\ &= \sigma_k(m-1, \ell) + C_k(z_m) \sigma_k(m-1, \ell-1), \end{aligned}$$

for $m \geq 2$ and $\ell \geq 2$. It is easy to see that $\sigma_k(1,1) = C_k(z_1)$. We also have

$$\sigma_k(m,1) = \sum_{j=1}^{m} C_k(z_j) \quad \text{and} \quad \sigma_k(m,m) = \prod_{j=1}^{m} C_k(z_j).$$

For each k, the quantities $\sigma_k(m,\ell)$ may be viewed as being the elements of a lower triangular matrix. Then to compute the quantities $\sigma_k(m,\ell)$ required for $e^2_{n,m}(z_1, z_2, \ldots, z_m)$, we can use the following algorithm (with $\sigma_k(1,1) = C_k(z_1)$):

Set $\sigma_k(m,1) = \sum_{j=1}^{m} C_k(z_j)$.
Set $\sigma_k(m,m) = \prod_{j=1}^{m} C_k(z_j)$.
For $\ell = 2, 3, \ldots, m-1$ do:

$$\sigma_k(m,\ell) = \sigma_k(m-1,\ell) + C_k(z_m)\sigma_k(m-1,\ell-1).$$

Now it is clear that if for each m, the quantities $\sigma_k(m-1,\ell)$ for $\ell = 1, 2, \ldots, m-1$ have been computed and stored using $O(m)$ memory, then the computation of all $\sigma_k(m,\ell)$ as well as of $\sum_{\ell=1}^{m} \Gamma_\ell \sigma_k(m,\ell)$ will require only $O(m)$ operations for each k, assuming that the values of $C_k(z_m)$ have also been stored as indicated in Section 2.7.1. Since there are n possible values for k, the amount of storage required is $O(nd)$ for a complete run of the algorithm. In conclusion, the computation of $e^2_{n,m}(z_1, z_2, \ldots, z_m)$ for each z_m requires $O(nm)$ operations, and the total cost of the CBC algorithm will be $O(n^2d^2)$. This shows that the complexity of the CBC construction is smaller for order-dependent weights than for finite-order weights.

2.7.4 The cost of the construction for weights which are both order-dependent and finite-order

If we assume that the order-dependent weights are also finite-order, then

$$e^2_{n,d}(\boldsymbol{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\ell=1}^{q^*} \Gamma_\ell \sigma_k(d,\ell).$$

With the assumption that $q^* < d$, the total cost of the construction will be reduced to $O(n^2dq^*)$, with additional $O(nq^*)$ memory required for storage.

2.7.5 Speeding up the CBC construction

A fast CBC construction has recently been proposed by Nuyens and Cools in [44] for shift-invariant reproducing kernel Hilbert spaces. Their technique is based on writing the CBC algorithm appropriate for these function spaces in terms of matrix-vector multiplications and then applying a fast algorithm to do these multiplications. For the multiplication of an $n \times n$ matrix with an n-vector, the operation count is reduced to $O(n \ln n)$ from the usual $O(n^2)$. In [44], the authors have shown that this reduction of the operation count is possible by using the special structure of the matrix occurring in the matrix-vector multiplication. Further details can be found in [44, Section 4].

Their technique can be modified so that it works for the CBC algorithm given in Section 2.4. Thus for the case of general weights, the $O(n^2 d 2^d)$ operation count may be reduced to $O(n \ln(n) d 2^d)$, while for finite-order weights the operation count may be reduced to $O(n \ln(n) d^{q^*+1})$.

In the case of order-dependent weights, we recall from Subsection 2.7.3 that

$$\sigma_k(m, \ell) = \sigma_k(m-1, \ell) + C_k(z_m)\sigma_k(m-1, \ell-1),$$

for $m \geq 2$ and $\ell \geq 2$. We also see that we can write $\sigma_k(m, 1) = \sigma_k(m-1, 1) + C_k(z_m)$ and $\sigma_k(m, m) = \sigma_k(m-1, m-1)C_k(z_m)$. Hence we can write

$$\begin{aligned}
e^2_{n,m}(z_1, z_2, \ldots, z_m) &= \frac{1}{n}\sum_{k=0}^{n-1}\sum_{\ell=1}^{m}\Gamma_\ell \sigma_k(m, \ell) \\
&= \frac{1}{n}\sum_{k=0}^{n-1}\left(\Gamma_1\sigma_k(m,1) + \sum_{\ell=2}^{m-1}\Gamma_\ell\sigma_k(m,\ell) + \Gamma_m\sigma_k(m,m)\right) \\
&= \frac{1}{n}\sum_{k=0}^{n-1}\Gamma_1(\sigma_k(m-1,1) + C_k(z_m)) \\
&\quad + \frac{1}{n}\sum_{k=0}^{n-1}\sum_{\ell=2}^{m-1}\Gamma_\ell(\sigma_k(m-1,\ell) + C_k(z_m)\sigma_k(m-1,\ell-1)) \\
&\quad + \frac{1}{n}\sum_{k=0}^{n-1}\Gamma_m C_k(z_m)\sigma_k(m-1,m-1) \\
&= e^2_{n,m-1}(z_1, z_2, \ldots, z_{m-1}) \\
&\quad + \frac{1}{n}\sum_{k=0}^{n-1} C_k(z_m)\left(\Gamma_1 + \sum_{\ell=2}^{m}\Gamma_\ell\sigma_k(m-1,\ell-1)\right).
\end{aligned}$$

The inner parenthesis can be computed in $O(m)$ operations for every k (with the σ_k's being stored), hence a total of $O(nm)$ operations. Let us denote

$$\boldsymbol{\sigma}(m,\ell) := [\sigma_k(m,\ell)]_{k\in\{0,1,\ldots,n-1\}}\,.$$

We also put $\sigma_k(0,0) = 1$ for all $k \in \{0,1,\ldots,n-1\}$. Now by denoting

$$\boldsymbol{e^2_{n,m}} = [e^2_{n,m}(z_1,z_2,\ldots,z_m)]_{z_m\in\{1,2,\ldots,n-1\}}$$

and

$$\boldsymbol{C}_n := [C_k(z_m)]_{\substack{z_m\in\{1,2,\ldots,n-1\}\\ k\in\{0,1,\ldots,n-1\}}}\,,$$

we then can write

$$\boldsymbol{e^2_{n,m}} = \boldsymbol{e^2_{n,m-1}} + \frac{1}{n}\boldsymbol{C}_n\left(\sum_{\ell=1}^{m}\Gamma_\ell\boldsymbol{\sigma}(m-1,\ell-1)\right).$$

By first doing a summation over all weights and then applying the fast matrix-vector multiplication (requiring $O(n\log n)$ operations), we find that the computational cost of the construction is $O(nm + n\log n)$ for every m. Hence the total complexity will be

$$\sum_{m=2}^{d} O(nm + n\log n) = O(nd^2 + nd\log n)$$

plus $O(nd)$ storage as mentioned in Section 2.7.3. Further details of such a fast algorithm can also be found in [6, Section 4]. In that work, a function of the form

$$\frac{1}{n}\sum_{k=0}^{n-1}\sum_{\ell=1}^{d}\Gamma_\ell\sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}\\|\mathfrak{u}|=\ell}}\prod_{j\in\mathfrak{u}}\omega\left(\left\{\frac{kz_j}{n}\right\}\right)$$

was minimised. For the weighted star discrepancy considered here, we see from Section 2.7.3 that we can apply their fast algorithm by taking

$$\omega\left(\left\{\frac{kz_j}{n}\right\}\right) = C_k(z_j) = \sum_{-\frac{n}{2}<h\le\frac{n}{2}}{}' \frac{e^{2\pi\mathrm{i}hkz_j/n}}{|h|}.$$

Finally, if the weights are both order-dependent and finite-order, then the cost of the construction will be $O(nd\ln(n) + ndq^*) = O(nd\ln n)$ with $O(nq^*)$ additional storage.

Chapter 3

Good intermediate-rank lattice rules based on the weighted star discrepancy

In this chapter we study the problem of constructing good intermediate-rank lattice rules in the sense of having a low weighted star discrepancy, where the weights are assumed to have a product form. The intermediate-rank rules considered here are obtained by "copying" rank-1 lattice rules. We show that such lattice rules can be constructed using a component-by-component technique and prove that the bound for the weighted star discrepancy achieves the optimal convergence rate.

3.1 Introduction

We want to approximate integrals over the d-dimensional unit cube given by intermediate-rank lattice rules of the form (see also (1.7))

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

where $\ell \geq 1$ is an integer satisfying $\gcd(\ell, n) = 1$, r is a fixed integer taken from the set $\{0, 1, \ldots, d\}$ and $N = \ell^r n$.

As mentioned in the first chapter, the rank of a lattice rule represents the minimal number of sums required to write it down. For d-dimensional integrals, lattice rules may have rank up to d. Further details on the definition and the representation of lattice rules can be found in [51] and [53]. For $r \geq 1$, (1.7) is a rank-r lattice rule or "intermediate-rank lattice rule" with $N = \ell^r n$ distinct points and is obtained by copying the rank-1 lattice rule (1.5) ℓ times in each of the first r dimensions. Here, $\boldsymbol{z} \in \mathbb{Z}^d$ is the generating vector having the same properties as mentioned in Chapter 2, that is, all the components of $\boldsymbol{z}$ are assumed to be relatively prime with n. In this chapter, we shall construct lattice rules of the form (1.7) by using a weighted star discrepancy as a criterion of goodness.

The intermediate-rank lattice rules considered here have been previously studied in [30], [37], [49], and [51]. In fact, the results from this chapter are based on the results obtained in [49].

3.2 Bounds for the weighted star discrepancy

We observe first that the quadrature points of the lattice rule (1.7) can be rewritten as:

$$\left\{ \frac{k\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell} \right\} = \frac{\boldsymbol{y}_t}{N},$$

where $\boldsymbol{y}_t/N$, $0 \leq t \leq N-1$, are in $[0,1)^d$. Of course, these points just are a reordering of the N-points of the rank-r lattice rule defined by (1.7). The set $\{\boldsymbol{y}_t/N,\ 0 \leq t \leq N-1\}$ will be denoted by P_N. Now let us introduce a set of non-increasing positive weights $\{\gamma_j\}_{j=1}^{\infty}$ which describe the decreasing importance of the successive coordinate directions. In such a case the weights are product, hence recall from (1.12) that the weights have the form

$$\boldsymbol{\gamma}_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j, \quad \forall \mathfrak{u} \subseteq \mathcal{D}.$$

As mentioned in the first chapter, product weights have been first used in [57]. Later, a similar assumption on the weights has been made in numerous

research papers including [8], [20], [29], [35], [36], [37], [38], [49], [50], [52], and [62].

From Zaremba's identity (see (2.1)) and by applying Hölder's inequality for integrals and sums, we obtain

$$\begin{aligned}\left|Q_{N,d}^{(r)}(f) - I_d(f)\right| &\leq \left(\sum_{\mathfrak{u}\subseteq\mathcal{D}} \sup_{\boldsymbol{x}_\mathfrak{u}\in[0,1]^{|\mathfrak{u}|}} \boldsymbol{\gamma}_\mathfrak{u} \left|\mathrm{discr}((\boldsymbol{x}_\mathfrak{u},\mathbf{1}),P_N)\right|\right) \\ &\times \sup_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_\mathfrak{u}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \left|\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_\mathfrak{u}} f((\boldsymbol{x}_\mathfrak{u},\mathbf{1}))\right| \mathrm{d}\boldsymbol{x}_\mathfrak{u}. \end{aligned} \tag{3.1}$$

Thus we can define a weighted star discrepancy $D^*_{N,\boldsymbol{\gamma}}(P_N)$ by

$$D^*_{N,\boldsymbol{\gamma}}(P_N) := \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_\mathfrak{u} \sup_{\boldsymbol{x}_\mathfrak{u}\in[0,1]^{|\mathfrak{u}|}} \left|\mathrm{discr}((\boldsymbol{x}_\mathfrak{u},\mathbf{1}),P_N)\right|. \tag{3.2}$$

Let us remark that (3.2) is different from the corresponding version of the weighted star discrepancy from Chapter 2. In fact, if we consider the weighted star discrepancy introduced in the previous chapter by (2.2), we see that (2.2) will be bounded by the right-hand-side of (3.2). This alternative way to define the weighted star discrepancy is important because it will allow us to obtain bounds on the L_p star discrepancy (details can be found in [29] and will also be given later in Section 3.6), while with the weighted star discrepancy (2.2) from the previous chapter, we were restricted only to the L_∞ case as attempts to obtain subsequent results for the L_p star discrepancy were not successful.

Define now the quantity

$$R_N(P_N,\mathfrak{u}) = \frac{1}{N}\sum_{t=0}^{N-1}\prod_{j\in\mathfrak{u}}\left(1 + {\sum_{-N/2<h\leq N/2}}' \frac{e^{2\pi \mathrm{i} h y_{t,j}/N}}{|h|}\right) - 1, \tag{3.3}$$

where $y_{t,j}$ is the j-th component of the vector $\boldsymbol{y}_t$. If L is the integration lattice associated with the points P_N, we denote by $L_\mathfrak{u}$ the $|\mathfrak{u}|$-dimensional lattice obtained from L by taking the coordinates that belong to $\mathfrak{u}$. Then, using Theorem 2.1 (see also (2.5)), we obtain:

$$R_N(P_N,\mathfrak{u}) = \sum_{\boldsymbol{h}\in L_\mathfrak{u}^\perp\cap E^*_{N,|\mathfrak{u}|}} \prod_{j\in\mathfrak{u}} \frac{1}{\max(1,|h_j|)}, \tag{3.4}$$

where we recall from the previous chapter (see (2.8)) that

$$E^*_{n,s} := \{\boldsymbol{h}\in\mathbb{Z}^s,\ \boldsymbol{h}\neq\mathbf{0} : -n/2 < h_j \leq n/2,\ 1\leq j\leq s\}.$$

From Theorem 2.2 and by applying (2.7), we obtain:

$$\begin{aligned}
&\sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_N)| \\
\leq\ & 1-(1-1/N)^{|\mathfrak{u}|} + \sum_{\boldsymbol{h}\in E^*_{N,|\mathfrak{u}|}} \frac{1}{\prod_{j\in\mathfrak{u}} r(h_j,N)} \left|\frac{1}{N}\sum_{t=0}^{N-1} e^{2\pi \mathrm{i}\boldsymbol{h}\cdot\boldsymbol{y}_{t,\mathfrak{u}}/N}\right| \\
=\ & 1-(1-1/N)^{|\mathfrak{u}|} + \sum_{\boldsymbol{h}\in L_{\mathfrak{u}}^{\perp}\cap E^*_{N,|\mathfrak{u}|}} \frac{1}{\prod_{j\in\mathfrak{u}} r(h_j,N)},
\end{aligned}$$

where $\boldsymbol{y}_{t,\mathfrak{u}}$ is the vector obtained from $\boldsymbol{y}_t$ by taking only the components that belong to $\mathfrak{u}$, while $r(h,N)$ was defined in Chapter 2 (see Theorem 2.2). By making use of $\sin\ \pi t \geq 2t$ for any $0\leq t\leq \frac{1}{2}$ (see also Theorem 2.3), we obtain:

$$\sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_N)| \leq 1-(1-1/N)^{|\mathfrak{u}|} + \frac{R_N(P_N,\mathfrak{u})}{2},$$

where $R_N(P_N,\mathfrak{u})$ is given by (3.4). Replacing in (3.2), we obtain the following bound:

$$D^*_{N,\boldsymbol{\gamma}}(P_N) \leq \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1-(1-1/N)^{|\mathfrak{u}|} + \frac{R_N(P_N,\mathfrak{u})}{2}\right). \tag{3.5}$$

We remark that since the points P_N are fully determined when $\boldsymbol{z}$ is known, it makes sense to denote the discrepancy $D^*_{N,\boldsymbol{\gamma}}(P_N)$ by $D^*_{N,\boldsymbol{\gamma}}(\boldsymbol{z})$ as it was also done in Chapter 2. Further bounds on the weighted star discrepancy may be obtained by making use of (3.5).

We first consider the quantity $\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}\left(1-(1-1/N)^{|\mathfrak{u}|}\right)$, which can be analysed in a similar way as in the proof of [29, Lemma 1]. This result is given next.

Lemma 3.1 *If the weights γ_j are summable (that is, $\sum_{j=1}^{\infty}\gamma_j<\infty$), then*

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}\left(1-(1-1/N)^{|\mathfrak{u}|}\right) \leq \frac{\max(1,\Gamma)}{\ell^r n} e^{\sum_{j=1}^{\infty}\gamma_j} = O(n^{-1}),$$

where $\Gamma := \sum_{j=1}^{\infty}\gamma_j/(1+\gamma_j)$ and the implied constant depends on ℓ, r and the weights but is independent of the dimension.

Proof. Recalling that the weights are product, we have

$$\begin{aligned}
\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}\left(1-(1-1/N)^{|\mathfrak{u}|}\right) &= \prod_{j=1}^{d}(1+\gamma_j) - \prod_{j=1}^{d}(1+\gamma_j(1-1/N)) \\
&= \prod_{j=1}^{d}(1+\gamma_j)\left[1-\prod_{j=1}^{d}\left(1-\frac{\gamma_j}{N(1+\gamma_j)}\right)\right].
\end{aligned}$$

Using the fact that the function $g(x) = \frac{\ln(1-x)}{x}$ is decreasing on $(0,1)$, then since $0 < \frac{\gamma_j}{N(1+\gamma_j)} \leq \frac{1}{N} < 1$, it is easy to check that

$$\ln\left(1 - \frac{\gamma_j}{N(1+\gamma_j)}\right) \geq \frac{\gamma_j}{1+\gamma_j} \ln(1-1/N).$$

This leads to

$$-\ln\left(\prod_{j=1}^{d}\left(1 - \frac{\gamma_j}{N(1+\gamma_j)}\right)\right) \leq -\ln(1-1/N) \sum_{j=1}^{d} \frac{\gamma_j}{1+\gamma_j}.$$

Let us remark that similar arguments have been used in [20]. We now obtain

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1 - (1-1/N)^{|\mathfrak{u}|}\right) \leq \prod_{j=1}^{d}(1+\gamma_j) \left[1 - \left(1 - \frac{1}{N}\right)^{\sum_{j=1}^{d} \gamma_j/(1+\gamma_j)}\right]. \quad (3.6)$$

Now note that since the weights γ_j are summable and $\gamma_j/(1+\gamma_j) < \gamma_j$, then $\Gamma := \sum_{j=1}^{\infty} \gamma_j/(1+\gamma_j) < \infty$. Now, if $\Gamma \leq 1$, then

$$1 - \left(1 - \frac{1}{N}\right)^{\Gamma} \leq 1 - \left(1 - \frac{1}{N}\right) = \frac{1}{N}.$$

If $\Gamma > 1$, then it can be easily verified that the function $f(x) = (1+x)^{\Gamma} - \Gamma x - 1 \geq 0$, for any $x > -1$ and hence $f(-1/N) \geq 0$. This leads to

$$\left(1 - \frac{1}{N}\right)^{\Gamma} + \frac{\Gamma}{N} - 1 \geq 0,$$

and so,

$$1 - \left(1 - \frac{1}{N}\right)^{\Gamma} \leq \frac{\Gamma}{N}.$$

Then from (3.6), we obtain:

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1 - (1-1/N)^{|\mathfrak{u}|}\right) \leq \frac{\max(1,\Gamma)}{N} \prod_{j=1}^{\infty}(1+\gamma_j) \leq \frac{\max(1,\Gamma)}{\ell^r n} e^{\sum_{j=1}^{\infty} \gamma_j},$$

where we used that

$$\prod_{j=1}^{\infty}(1+\gamma_j) = e^{\sum_{j=1}^{\infty} \ln(1+\gamma_j)} \leq e^{\sum_{j=1}^{\infty} \gamma_j},$$

with the last step following from $\ln(1+x) \leq x$, for any $x > -1$. □

We next consider the quantity $\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}R_N(P_N,\mathfrak{u})$ that occurs in the right-hand-side of (3.5). By making use of (3.3) and (2.14), we obtain:

$$\begin{aligned}
\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}R_N(P_N,\mathfrak{u}) &= \sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\left[\frac{1}{N}\sum_{t=0}^{N-1}\prod_{j\in\mathfrak{u}}\left(1+\sum_{-N/2<h\leq N/2}{}'\frac{e^{2\pi\mathrm{i}hy_{t,j}/N}}{|h|}\right)-1\right]\\
&= \sum_{\mathfrak{u}\subseteq\mathcal{D}}\left[\frac{1}{N}\sum_{t=0}^{N-1}\prod_{j\in\mathfrak{u}}\gamma_j\left(1+\sum_{-N/2<h\leq N/2}{}'\frac{e^{2\pi\mathrm{i}hy_{t,j}/N}}{|h|}\right)\right]\\
&\quad -\sum_{\mathfrak{u}\subseteq\mathcal{D}}\prod_{j\in\mathfrak{u}}\gamma_j\\
&= \frac{1}{N}\sum_{t=0}^{N-1}\prod_{j=1}^{d}\left(1+\gamma_j+\gamma_j\sum_{-N/2<h\leq N/2}{}'\frac{e^{2\pi\mathrm{i}hy_{t,j}/N}}{|h|}\right)\\
&\quad -\prod_{j=1}^{d}(1+\gamma_j).
\end{aligned}$$

Let's remark that a similar analysis has been used in [29] for rank-1 lattice rules. If we denote $\beta_j=1+\gamma_j$ and set

$$e^2_{N,d}(\boldsymbol{z}):=\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}R_N(P_N,\mathfrak{u}),$$

then we obtain

$$e^2_{N,d}(\boldsymbol{z})=\frac{1}{N}\sum_{t=0}^{N-1}\prod_{j=1}^{d}\left(\beta_j+\gamma_j\sum_{-\frac{N}{2}<h\leq\frac{N}{2}}{}'\frac{e^{2\pi\mathrm{i}hy_{t,j}/N}}{|h|}\right)-\prod_{j=1}^{d}\beta_j. \tag{3.7}$$

Let's remark that the dependency on $\boldsymbol{z}$ in $e^2_{N,d}(\boldsymbol{z})$ makes sense as the vectors $\boldsymbol{y}_t$ actually depend on $\boldsymbol{z}$. In research papers such as [27] or [30], it was proved that when n is prime, the quantity (3.7) is identical to a quadrature error obtained from applying a rank-1 lattice rule to a certain integrand. Working with such a quadrature error simplifies in general the analysis of the problem. Indeed, from (1.7) and (3.7) we have

$$\begin{aligned}
e^2_{N,d}(\boldsymbol{z}) &= \frac{1}{n}\sum_{k=0}^{n-1}\frac{1}{\ell^r}\sum_{m_r=0}^{\ell-1}\cdots\sum_{m_1=0}^{\ell-1}\prod_{j=1}^{r}\left(\beta_j+\gamma_j\sum_{-\frac{N}{2}<h\leq\frac{N}{2}}{}'\frac{e^{2\pi\mathrm{i}h(kz_j/n+m_j/\ell)}}{|h|}\right)\\
&\quad\times\prod_{j=r+1}^{d}\left(\beta_j+\gamma_j\sum_{-\frac{N}{2}<h\leq\frac{N}{2}}{}'\frac{e^{2\pi\mathrm{i}hkz_j/n}}{|h|}\right)-\prod_{j=1}^{d}\beta_j\\
&= \frac{1}{n}\sum_{k=0}^{n-1}A_k^{(\ell,r)}\prod_{j=r+1}^{d}\left(\beta_j+\gamma_j\sum_{-\frac{N}{2}<h\leq\frac{N}{2}}{}'\frac{e^{2\pi\mathrm{i}hkz_j/n}}{|h|}\right)-\prod_{j=1}^{d}\beta_j,
\end{aligned}$$

where

$$A_k^{(\ell,r)} = \frac{1}{\ell^r} \sum_{m_r=0}^{\ell-1} \cdots \sum_{m_1=0}^{\ell-1} \prod_{j=1}^{r} \left(\beta_j + \gamma_j \sum_{-\frac{N}{2}<h\le\frac{N}{2}}{}' \frac{e^{2\pi \mathrm{i} h(kz_j/n + m_j/\ell)}}{|h|} \right).$$

Before expanding $A_k^{(\ell,r)}$, let's also observe that (2.22) leads to

$$\sum_{m=0}^{\ell-1} \left(e^{2\pi \mathrm{i} h/\ell}\right)^m = \begin{cases} \ell, & h \equiv 0 \,(\mathrm{mod}\, \ell), \\ 0, & \text{otherwise.} \end{cases}$$

Then we have

$$\begin{aligned} A_k^{(\ell,r)} &= \prod_{j=1}^{r} \frac{1}{\ell} \sum_{m=0}^{\ell-1} \left(\beta_j + \gamma_j \sum_{-\frac{N}{2}<h\le\frac{N}{2}}{}' \frac{e^{2\pi \mathrm{i} h(kz_j/n + m/\ell)}}{|h|} \right) \\ &= \prod_{j=1}^{r} \frac{1}{\ell} \sum_{m=0}^{\ell-1} \left(\beta_j + \gamma_j \sum_{-\frac{N}{2}<h\le\frac{N}{2}}{}' \frac{e^{2\pi \mathrm{i} hkz_j/n}}{|h|} \left(e^{2\pi \mathrm{i} h/\ell}\right)^m \right) \\ &= \prod_{j=1}^{r} \frac{1}{\ell} \left(\ell\beta_j + \ell\gamma_j \sum_{\substack{-\frac{N}{2}<h\le\frac{N}{2} \\ h\equiv 0 \,(\mathrm{mod}\, \ell)}}{}' \frac{e^{2\pi \mathrm{i} hkz_j/n}}{|h|} \right) \\ &= \prod_{j=1}^{r} \left(\beta_j + \gamma_j \sum_{-\frac{N}{2}<q\ell\le\frac{N}{2}}{}' \frac{e^{2\pi \mathrm{i} q\ell kz_j/n}}{|q|\ell} \right) \\ &= \prod_{j=1}^{r} \left(\beta_j + \frac{\gamma_j}{\ell} \sum_{-\frac{N}{2\ell}<h\le\frac{N}{2\ell}}{}' \frac{e^{2\pi \mathrm{i} h\ell kz_j/n}}{|h|} \right). \end{aligned}$$

Going back to the expression for $e_{N,d}^2(\boldsymbol{z})$, we obtain

$$e_{N,d}^2(\boldsymbol{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_j/n}}{|h|} \right) - \prod_{j=1}^{d} \beta_j, \tag{3.8}$$

where the following notations have been introduced:

$$\tilde{\gamma}_j = \begin{cases} \gamma_j/\ell, & 1 \le j \le r, \\ \gamma_j, & r+1 \le j \le d. \end{cases} \tag{3.9}$$

Next,

$$\tilde{N}_j = \begin{cases} N/\ell = \ell^{r-1} n, & 1 \le j \le r, \\ N, & r+1 \le j \le d. \end{cases} \tag{3.10}$$

Finally, $\hat{\boldsymbol{z}} = (\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_d)$, with

$$\hat{z}_j = \begin{cases} \ell z_j, & 1 \le j \le r, \\ z_j, & r+1 \le j \le d. \end{cases} \tag{3.11}$$

Then by denoting

$$f_N(\boldsymbol{x}) = \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h x_j}}{|h|} \right),$$

it is easy to observe that

$$e^2_{N,d}(\boldsymbol{z}) = \frac{1}{n} \sum_{k=0}^{n-1} f_N\left(\frac{k}{n}\hat{\boldsymbol{z}}\right) - \prod_{j=1}^{d} \beta_j.$$

Now it is clear that $e^2_{N,d}(\boldsymbol{z})$ (which is based on a rank-r lattice rule with $N = \ell^r n$ points) can be obtained from applying a modified n-point rank-1 lattice rule to f_N.

Next, we seek to obtain a result for the mean of the quantities $e^2_{N,d}(\boldsymbol{z})$. Such a result, together with (3.5) and Lemma 3.1, will allow us to deduce a certain bound for the weighted star discrepancy. This mean will be taken over all possible values of $\hat{\boldsymbol{z}}$. Because $\hat{\boldsymbol{z}}$ is known when $\boldsymbol{z}$ is known, the mean will be actually considered for all possible values for $\boldsymbol{z}$. As mentioned already in Chapter 2, each component z_j of the vector $\boldsymbol{z}$ can be taken from the set $\mathcal{Z}_n = \{1, 2, \ldots, n-1\}$ for any $1 \le j \le d$. Thus, for prime n, the mean $M_{N,d,\boldsymbol{\gamma}}$ is defined by

$$M_{N,d,\boldsymbol{\gamma}} := \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} e^2_{N,d}(\boldsymbol{z}).$$

An expression for $M_{N,d,\boldsymbol{\gamma}}$ is given in the next theorem.

Theorem 3.2 *If n is prime, ℓ is a positive integer such that $gcd(\ell, n) = 1$ and r is an integer chosen such that $1 \le r \le d$, then*

$$\begin{aligned} M_{N,d,\gamma} &= \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j} \right) \\ &+ \frac{n-1}{n} \prod_{j=1}^{d} \left(\beta_j - \frac{\tilde{\gamma}_j}{n-1} \left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n} \right) \right) - \prod_{j=1}^{d} \beta_j, \end{aligned} \tag{3.12}$$

where we recall from Chapter 2 that

$$S_m = \sum_{-\frac{m}{2} \le h < \frac{m}{2}}{}' \frac{1}{|h|}.$$

Proof. Using the definition of the mean and separating out the $k = 0$ term from (3.8), we obtain:

$$M_{N,d,\gamma} = \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j} \right) + \Theta_{N,d,\gamma} - \prod_{j=1}^{d} \beta_j, \tag{3.13}$$

where

$$\begin{aligned}
\Theta_{N,d,\gamma} &= \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} \left(\frac{1}{n} \sum_{k=1}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j / n}}{|h|} \right) \right) \\
&= \frac{1}{n} \sum_{k=1}^{n-1} \prod_{j=1}^{d} \left(\frac{1}{n-1} \sum_{z_j=1}^{n-1} \left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j / n}}{|h|} \right) \right) \\
&= \frac{1}{n} \sum_{k=1}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \frac{\tilde{\gamma}_j}{n-1} \sum_{z_j=1}^{n-1} \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j / n}}{|h|} \right).
\end{aligned}$$

For $1 \le k \le n-1$ and for any $j \ge 1$, consider now

$$T_n(k,j) = \frac{1}{n-1} \sum_{z_j=1}^{n-1} \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j / n}}{|h|}. \tag{3.14}$$

If $1 \le j \le r$, then $\hat{z}_j = \ell z_j$. Since $\gcd(\ell, n) = 1$, it follows that for any $1 \le j \le d$, we can write $e^{2\pi \mathrm{i} h k \hat{z}_j / n} = e^{2\pi \mathrm{i} h q z_j / n}$ for some $q \in \{1, 2, \ldots, n-1\}$ and hence $T_n(k,j) = T_{\tilde{N}_j}(q)$, where $T_{\tilde{N}_j}(q)$ is as defined by (2.20). By applying Lemma 2.5, we obtain

$$T_n(k,j) = \frac{S_{\tilde{N}_j/n} - S_{\tilde{N}_j}}{n-1}, \tag{3.15}$$

for any $1 \le k \le n-1$ and for any $1 \le j \le d$. Using now (3.15), we see that

$$\Theta_{N,d,\gamma} = \frac{1}{n} \sum_{k=1}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \frac{\tilde{\gamma}_j}{n-1} \left(S_{\tilde{N}_j/n} - S_{\tilde{N}_j} \right) \right),$$

and by replacing in (3.13), we obtain the desired result. □

From this theorem, we can deduce the following:

Corollary 3.3 *If n is prime, ℓ is a positive integer such that $gcd(\ell, n) = 1$ and r satisfies $1 \le r \le d$, then there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$e_{N,d}^2(\boldsymbol{z}) \le \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) \le \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + 2\tilde{\gamma}_j \ln \tilde{N}_j\right).$$

Proof. In order to obtain the desired bound for $e_{N,d}^2(\boldsymbol{z})$, we see from (3.13) that it will suffice to prove that

$$\Theta_{N,d,\gamma} \le \prod_{j=1}^{d} \beta_j,$$

together with the argument that there must be a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that

$$e_{N,d}^2(\boldsymbol{z}) \le M_{N,d,\gamma}.$$

From Lemma 2.9 (see also [41, Lemmas 1 and 2]), we deduce that

$$S_{\tilde{N}_j} - S_{\tilde{N}_j/n} < 2 \ln n + \frac{1}{\tilde{N}_j^2} + \frac{4}{(\tilde{N}_j/n)^2}. \tag{3.16}$$

If $\ell = 1$, then the intermediate-rank considered in this chapter is actually a rank-1 lattice rule with n points. For rank-1 lattice rules, the corresponding result has been proved in [29, Corollary 1]. So it makes sense to assume that $\ell \ge 2$. Next, we verify that for any $1 \le j \le d$, we have

$$\left|\beta_j - \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right)\right| \le \beta_j. \tag{3.17}$$

The inequality $\beta_j - \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right) \le \beta_j$ is trivial. It remains to prove that $\beta_j - \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right) \ge -\beta_j$, which is equivalent with

$$2\beta_j = 2 + 2\gamma_j \ge \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right).$$

Let us take first $r = 1$. Then $1 \le j \le r$ implies that $j = 1$ and in this case we deduce that $S_{\tilde{N}_1} - S_{\tilde{N}_1/n} = S_n$. Hence the inequality above is equivalent with

$$2 + 2\gamma_1 \ge \frac{\tilde{\gamma}_1 S_n}{n-1}.$$

Since $S_n \le 2 \ln n$ (see Corollary 2.10), we have

$$\frac{\tilde{\gamma}_1 S_n}{n-1} \le \frac{2\gamma_1 \ln n}{\ell(n-1)} \le 2 + 2\gamma_1,$$

where the last step follows from $\ln n \leq n-1$ for any $n \geq 1$. Consequently, (3.17) will hold. If $r \geq 2$, we can prove that

$$2\gamma_j \geq \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right),$$

for any $1 \leq j \leq d$. If $\ell = 2$ then since $\gcd(\ell, n) = 1$, it follows that $n \geq 3$. It is easy to see that the right-hand-side of (3.16) can be further bounded so that we obtain

$$\frac{\tilde{\gamma}_j(S_{\tilde{N}_j} - S_{\tilde{N}_j/n})}{n-1} \leq \frac{\gamma_j(2\ln n + 1 + 1/36)}{n-1} \leq 2\gamma_j,$$

for any $1 \leq j \leq d$. If $n = 2$, then since $\gcd(\ell, n) = 1$, it must follow that $\ell \geq 3$ and a simple direct calculation will show that the right-hand-side of (3.16) is further bounded by $2\ln 2 + 1/36 + 4/9 \leq 2$. This is enough to ensure that (3.17) holds also in this case. All these arguments lead to

$$\frac{n-1}{n}\prod_{j=1}^{d}\left(\beta_j - \frac{\tilde{\gamma}_j}{n-1}\left(S_{\tilde{N}_j} - S_{\tilde{N}_j/n}\right)\right) - \prod_{j=1}^{d}\beta_j \leq 0.$$

This inequality together with (3.12) and (2.24) then yields

$$M_{N,d,\gamma} \leq \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) \leq \frac{1}{n}\prod_{j=1}^{d}\left(\beta_j + 2\tilde{\gamma}_j \ln \tilde{N}_j\right),$$

which completes the proof. □

3.3 Strong tractability

From (3.5), Lemma 3.1 and Corollary 3.3, it follows that if the weights are summable, then there exists a generating vector $\boldsymbol{z}$ such that

$$D^*_{N,\gamma}(\boldsymbol{z}) \leq O(n^{-1}) + \frac{1}{2n}\prod_{j=1}^{d}\left(\beta_j + 2\tilde{\gamma}_j \ln \tilde{N}_j\right). \tag{3.18}$$

As the bound given by (3.18) has a $\ln n$ dependency (via the $\tilde{N}_j$), it would appear that the weighted star discrepancy has the order of magnitude of $O(n^{-1}(\ln n)^d)$, with the involved constant depending on d, ℓ and r. Without further assumptions over the weights, this leads to intractability. As we mentioned in Chapter 2, the order of magnitude $O(n^{-1}(\ln n)^d)$ is widely believed

to be the best possible in an unweighted setting (see [34], [39] or [42] for further details). However, under the assumption that the weights are summable, we can prove a strong tractability result (recall that tractability and strong tractability were introduced by Definition 1.6 and Definition 1.7). Such a result follows from the arguments in [20, Lemma 3] with some modifications and is presented below:

Theorem 3.4 *Let us assume that the weights γ_j are summable, that is*

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

Then for any $\delta > 0$, there exists a constant $C(\boldsymbol{\gamma}, \delta, \ell, r) > 0$, independent of n and d, such that

$$\prod_{j=1}^{d} \left(\beta_j + 2\tilde{\gamma}_j \ln \tilde{N}_j\right) \leq C(\boldsymbol{\gamma}, \delta, \ell, r)\ n^{\delta} e^{\sum_{j=1}^{\infty} \gamma_j}.$$

Proof. Recalling that $\beta_j = 1 + \gamma_j$, we see that we have

$$\prod_{j=1}^{d} \left(\beta_j + 2\tilde{\gamma}_j \ln \tilde{N}_j\right) \leq \left(\prod_{j=1}^{\infty} (1 + \gamma_j)\right) \times \left(\prod_{j=1}^{\infty} \left(1 + \overline{\gamma}_j \ln \tilde{N}_j\right)\right),$$

where $\overline{\gamma}_j = 2\tilde{\gamma}_j/(1 + \gamma_j)$, for each j. Now let us denote

$$\sigma_m = \sum_{j=m+1}^{\infty} \overline{\gamma}_j.$$

Because the γ_j are summable, we see that the weights $\overline{\gamma}_j$ are also summable since $\tilde{\gamma}_j/(1 + \gamma_j) \leq \gamma_j$ for each j. It is clear that σ_m may be made arbitrarily small by taking m sufficiently large. The condition of summability of the weights leads to

$$\prod_{j=1}^{\infty} (1 + \gamma_j) = \exp\left(\sum_{j=1}^{\infty} \ln(1 + \gamma_j)\right) \leq \exp\left(\sum_{j=1}^{\infty} \gamma_j\right) < \infty.$$

Since γ_j are all positive, we have $\sigma_m > 0$. Then

$$\begin{aligned}
\ln\left(\prod_{j=1}^{\infty}\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right)\right) &= \sum_{j=1}^{\infty} \ln\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right) \\
&\le \sum_{j=1}^{m} \ln\left(1+\sigma_m^{-1}+\overline{\gamma}_j \ln \tilde{N}_j\right) \\
&\quad + \sum_{j=m+1}^{\infty} \ln\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right) \\
&= \sum_{j=1}^{m} \ln\left(1+\sigma_m^{-1}\right) + \sum_{j=1}^{m} \ln\left(1+\frac{\overline{\gamma}_j \ln \tilde{N}_j}{1+\sigma_m^{-1}}\right) \\
&\quad + \sum_{j=m+1}^{\infty} \ln\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right) \\
&= m \ln\left(1+\sigma_m^{-1}\right) + \sum_{j=1}^{m} \ln\left(1+\frac{\overline{\gamma}_j \ln \tilde{N}_j}{1+\sigma_m^{-1}}\right) \\
&\quad + \sum_{j=m+1}^{\infty} \ln\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right).
\end{aligned}$$

Now since $\tilde{N}_j \le N$ for any j, we obtain

$$\begin{aligned}
\ln\left(\prod_{j=1}^{\infty}\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right)\right) &\le m \ln\left(1+\sigma_m^{-1}\right) + \sum_{j=1}^{m} \frac{\overline{\gamma}_j \sigma_m \ln \tilde{N}_j}{(1+\sigma_m^{-1})\sigma_m} \\
&\quad + \sum_{j=m+1}^{\infty} \overline{\gamma}_j \ln \tilde{N}_j \\
&\le m \ln\left(1+\sigma_m^{-1}\right) + \ln(N)\sigma_m \sum_{j=1}^{m} \overline{\gamma}_j + \ln(N)\sigma_m \\
&\le m \ln\left(1+\sigma_m^{-1}\right) + \ln(N)\sigma_m \left(\sigma_0+1\right).
\end{aligned}$$

Hence we have

$$\prod_{j=1}^{\infty}\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right) \le \left(1+\sigma_m^{-1}\right)^m N^{\sigma_m(\sigma_0+1)}.$$

By choosing m such that $\sigma_m(\sigma_0+1) \le \delta$, we obtain

$$\prod_{j=1}^{\infty}\left(1+\overline{\gamma}_j \ln \tilde{N}_j\right) \le \left(1+\sigma_m^{-1}\right)^m \ell^{r\delta} n^{\delta}.$$

Now, by taking $C(\boldsymbol{\gamma}, \delta, \ell, r) = (1+\sigma_m^{-1})^m \ell^{r\delta}$, we obtain the desired result. $\square$

From (3.18) and Theorem 3.4 we can conclude that there exists a generating vector $\boldsymbol{z}$ such that the weighted star discrepancy achieves the error bound

$$D^*_{N,\boldsymbol{\gamma}}(\boldsymbol{z}) = O(n^{-1+\delta}),$$

for any $\delta > 0$, where the implied constant depends on δ, ℓ, r and the weights but is independent of n and d. As mentioned in Chapter 1, since the bound on the discrepancy is independent of the dimension, this will ensure strong tractability.

3.4 Component-by-component construction of the generating vector

In this section we show that we can use the component-by component (CBC) construction so that the resulting intermediate-rank lattice rule has a bound on the weighted star discrepancy of the same order of magnitude as the bound given by Corollary 3.3. The CBC technique has been explained in Sections 1.4 and 2.4 and is based on the following algorithm:

Component-by-component (CBC) algorithm

The generating vector $\boldsymbol{z} = (z_1, z_2, \ldots, z_d)$ of an intermediate-rank lattice rule (1.7) can be constructed as follows:

1. Set the value for the first component of the vector, say $z_1 := 1$.

2. For $m = 2, 3, \ldots, d$, find $z_m \in \mathcal{Z}_n$ such that $e^2_{N,m}(z_1, z_2, \ldots, z_m)$ is minimised, where

$$e^2_{N,m}(z_1, z_2, \ldots, z_m) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{m}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\leq\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j/n}}{|h|}\right) - \prod_{j=1}^{m}\beta_j.$$

In order to justify the CBC algorithm, we next prove the following:

Theorem 3.5 *Let n be a prime, ℓ a positive integer such that $gcd(\ell, n) = 1$ and r be chosen such that $1 \leq r \leq d$. Assume there exists a vector $\boldsymbol{z}$ in $\mathcal{Z}_n^d$ such that*

$$e^2_{N,d}(\boldsymbol{z}) \leq \frac{1}{n-1}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right).$$

Then there exists a $z_{d+1} \in Z_n$ such that:

$$e^2_{N,d+1}(\boldsymbol{z}, z_{d+1}) \leq \frac{1}{n-1}\prod_{j=1}^{d+1}\left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right).$$

Such a z_{d+1} can be found by minimising $e^2_{N,d+1}(\boldsymbol{z}, z_{d+1})$ over $\mathcal{Z}_n$.

Proof. When we add a new component, we obtain from (3.8) that

$$\begin{aligned} e^2_{N,d+1}(\boldsymbol{z}, z_{d+1}) &= \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d+1}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\leq\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_j/n}}{|h|}\right) - \prod_{j=1}^{d+1}\beta_j \\ &= \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\leq\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_j/n}}{|h|}\right) \\ &\quad \times \left(\beta_{d+1} + \tilde{\gamma}_{d+1} \sum_{-\frac{\tilde{N}_{d+1}}{2}<h\leq\frac{\tilde{N}_{d+1}}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_{d+1}/n}}{|h|}\right) - \prod_{j=1}^{d+1}\beta_j. \end{aligned}$$

By separating out the $k=0$ term and by using (3.8), we see that we can write

$$\begin{aligned} e^2_{N,d+1}(\boldsymbol{z}, z_{d+1}) &= \beta_{d+1}e^2_{N,d}(\boldsymbol{z}) + \frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) \\ &\quad + \frac{\tilde{\gamma}_{d+1}}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\leq\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_j/n}}{|h|}\right) \\ &\quad \times \left(\sum_{-\frac{\tilde{N}_{d+1}}{2}<h\leq\frac{\tilde{N}_{d+1}}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_{d+1}/n}}{|h|}\right). \end{aligned}$$

We next average $e^2_{N,d+1}(\boldsymbol{z}, z_{d+1})$ over all possible values of $z_{d+1} \in \mathcal{Z}_n$ and consider:

$$\mathrm{Avg}(e^2_{N,d+1}(\boldsymbol{z}, z_{d+1})) = \frac{1}{n-1}\sum_{z_{d+1}=1}^{n-1} e^2_{N,d+1}(\boldsymbol{z}, z_{d+1}).$$

Since in the expression for the average, the last term is the only one depending on z_{d+1}, we next focus on the quantity

$$\frac{1}{n-1}\sum_{z_{d+1}=1}^{n-1}\sum_{-\frac{\tilde{N}_{d+1}}{2}<h\leq\frac{\tilde{N}_{d+1}}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_{d+1}/n}}{|h|} = \frac{1}{n-1}\left(S_{\tilde{N}_{d+1}/n} - S_{\tilde{N}_{d+1}}\right),$$

where the last equality was obtained by making use of (3.14) and (3.15). Substituting this in the expression for the average, we see that $\mathrm{Avg}(e^2_{N,d+1}(\boldsymbol{z}, z_{d+1}))$ is given by:

$$\begin{aligned} &\beta_{d+1}e^2_{N,d}(\boldsymbol{z}) + \frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) \\ &+ \frac{\tilde{\gamma}_{d+1}(S_{\tilde{N}_{d+1}} - S_{\tilde{N}_{d+1}/n})}{n(n-1)} \times \left[-\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\leq\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} hk\hat{z}_j/n}}{|h|}\right)\right]. \end{aligned}$$

Next,

$$\begin{aligned}
& -\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j\sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}'\frac{e^{2\pi \mathrm{i}hk\hat{z}_j/n}}{|h|}\right)\\
= & -\frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j\sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}'\frac{e^{2\pi \mathrm{i}hk\hat{z}_j/n}}{|h|}\right)+\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\\
= & -e^2_{N,d}(\boldsymbol{z})-\prod_{j=1}^{d}\beta_j+\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\le\frac{1}{n}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right).
\end{aligned}$$

In the last step we used $e^2_{N,d}(\boldsymbol{z})\ge 0$, as $R_N(P_N,\mathfrak{u})\ge 0$ for any $\mathfrak{u}\subseteq\mathcal{D}$ (see (3.4)). The hypothesis together with the obvious $S_{\tilde{N}_{d+1}}-S_{\tilde{N}_{d+1}/n}\le S_{\tilde{N}_{d+1}}$ lead us to:

$$\begin{aligned}
& \mathrm{Avg}(e^2_{N,d+1}(\boldsymbol{z},z_{d+1}))\\
\le\ & \beta_{d+1}e^2_{N,d}(\boldsymbol{z})+\frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\\
& +\frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n(n-1)}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\\
= & \beta_{d+1}e^2_{N,d}(\boldsymbol{z})+\frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\left(1+\frac{1}{n-1}\right)\\
\le\ & \frac{\beta_{d+1}}{n-1}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)+\frac{\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}}{n-1}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\\
= & \frac{1}{n-1}\prod_{j=1}^{d}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right)\left(\beta_{d+1}+\tilde{\gamma}_{d+1}S_{\tilde{N}_{d+1}}\right).
\end{aligned}$$

Clearly, the $z_{d+1}\in\mathcal{Z}_n$ chosen to minimise $e^2_{N,d+1}(\boldsymbol{z},z_{d+1})$ will satisfy

$$e^2_{N,d+1}(\boldsymbol{z},z_{d+1})\le\mathrm{Avg}(e^2_{N,d+1}(\boldsymbol{z},z_{d+1})).$$

This, together with the previous inequality completes the proof. □

From this theorem we can deduce the following:

Corollary 3.6 *Let n be prime, ℓ a positive integer such that $gcd(\ell,n)=1$ and r be chosen such that $1\le r\le d$. Then for any $m=1,2,\ldots,d$, there exists a $\boldsymbol{z}\in\mathcal{Z}_n^m$ such that*

$$e^2_{N,m}(z_1,z_2,\ldots,z_m)\le\frac{1}{n-1}\prod_{j=1}^{m}\left(\beta_j+\tilde{\gamma}_j S_{\tilde{N}_j}\right).$$

We can set $z_1 = 1$ and for every $2 \le m \le d$, z_m can be chosen by minimising $e^2_{N,m}(z_1, z_2, \ldots, z_m)$ over the set $\mathcal{Z}_n$.

Proof. If $m = 1$, then by expanding the expression for $e^2_{N,1}(z_1)$, we obtain:

$$\begin{aligned} e^2_{N,1}(z_1) &= \frac{1}{n}\sum_{k=0}^{n-1}\left(\beta_1 + \tilde{\gamma}_1 \sum_{-\frac{\tilde{N}_1}{2}<h\le\frac{\tilde{N}_1}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_1/n}}{|h|}\right) - \beta_1 \\ &= \frac{\tilde{\gamma}_1}{n}\sum_{k=0}^{n-1} \sum_{-\frac{\tilde{N}_1}{2}<h\le\frac{\tilde{N}_1}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_1/n}}{|h|} \\ &= \frac{\tilde{\gamma}_1}{n}\sum_{k=0}^{n-1}\left(\sum_{\substack{-\frac{\tilde{N}_1}{2}<h\le\frac{\tilde{N}_1}{2} \\ h\equiv 0 \,(\bmod\, n)}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_1/n}}{|h|} + \sum_{\substack{-\frac{\tilde{N}_1}{2}<h\le\frac{\tilde{N}_1}{2} \\ h\not\equiv 0 \,(\bmod\, n)}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_1/n}}{|h|}\right). \end{aligned}$$

Using now similar arguments as in the proof of Lemma 2.5, it follows that

$$e^2_{N,1}(z) = \frac{\tilde{\gamma}_1 S_{\tilde{N}_1/n}}{n} \le \frac{1}{n-1}\left(\beta_1 + \tilde{\gamma}_1 S_{\tilde{N}_1}\right),$$

for any $z_1 \in \mathcal{Z}_n$ and the desired inequality is proved for $d = 1$. The result then follows straight from Theorem 3.5. □

3.5 Computational costs incurred by the CBC algorithm

Let us first recall from the previous section that

$$e^2_{N,m}(z_1, z_2, \ldots, z_m) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{m}\left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j/n}}{|h|}\right) - \prod_{j=1}^{m}\beta_j.$$

Clearly each $e^2_{N,m}(z_1, z_2, \ldots, z_m)$ can be evaluated in $O(Nnm)$ operations. This cost can be reduced to $O(nm)$ by using additional storage. Since $\{k\hat{z}_j/n\} = q/n$ for some q satisfying $0 \le q \le n-1$, then, in a similar way as shown in Subsection 2.7.1, it will be enough to calculate each quantity

$$\sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h q/n}}{|h|}$$

once and then store it. From Appendix A, it follows that asymptotic expansion techniques similar to those in [31] (see also [29]) allow us to calculate the values of $F_N(q/n), 0 \le q \le n-1$, where

$$F_N(x) = \sum_{-N/2<h\le N/2}{}' \frac{e^{2\pi \mathrm{i} h x}}{|h|}, \quad 0 \le x \le 1,$$

at a total cost of $O(N)$ operations. For the intermediate-rank lattice rules considered in this chapter, we actually need the values of $F_{\tilde{N}_j}(q/n)$ when $\tilde{N}_j = \ell^r n$ and $\tilde{N}_j = \ell^{r-1} n$ (these are the only possible values for $\tilde{N}_j$). Once these quantities have been computed (in $O(N)$ operations), they can be stored in $O(n)$ memory locations.

It follows that the total complexity of the algorithm will be $O(n^2 d^2 + N)$ plus storage as indicated above. However since $N = \ell^r n$ and ℓ and r are fixed, we see that $N = O(n)$ and the complexity of the algorithm becomes $O(n^2 d^2)$ plus storage. We now observe that during the construction, we can also store the products involved in the expression for $e^2_{N,m}(\boldsymbol{z})$ for each $2 \le m \le d$. It turns out that the total cost of storage would be $O(n)$ for the quantities $F_{\tilde{N}_j}(q/n)$ and $O(n)$ for the products. Thus, the total computational cost of the algorithm is $O(n^2 d)$ plus storage.

Now, the fast CBC algorithm proposed by Nuyens and Cools in [44] can also be used here so that the computational cost of the CBC algorithm can be further reduced to $O(nd \log n)$. The approach in [44] was based on minimising a function of the form

$$\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(1 + \gamma_j \omega\left(\left\{\frac{k z_j}{n}\right\}\right)\right) - 1,$$

where ω is some function. Here, we can take

$$\omega\left(\left\{\frac{k z_j}{n}\right\}\right) = \sum_{-\frac{\tilde{N}_j}{2}<h\le\frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j/n}}{|h|}.$$

From (3.8), we know that $e^2_{N,d}(\boldsymbol{z})$ is obtained by applying a rank-1 lattice rule to a certain function, so the techniques used in [44] will also work here with some modifications.

3.6 Bounds for the weighted L_p discrepancy

This section is actually based on the results from [29, Section 4] and we shall see next that these results can be easily adapted so that they also work for the intermediate-rank lattice rules considered in this chapter.

Let's consider first two numbers $p, q \geq 1$ such that $1/p + 1/q = 1$. Then the L_p version of the weighted star discrepancy could be defined by

$$D^*_{N,\boldsymbol{\gamma},p}(\boldsymbol{z}) := \left(\sum_{\mathrm{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathrm{u}}^p \int_{[0,1]^{|u|}} |\mathrm{discr}((\boldsymbol{x}_{\mathrm{u}}, \mathbf{1}), P_N)|^p \, \mathrm{d}\boldsymbol{x}_{\mathrm{u}} \right)^{1/p}.$$

From Zaremba's identity (see (2.1)) and applying Hölder's inequality for integrals and sums, we can deduce that

$$\left| Q^{(r)}_{N,d}(f) - I_d(f) \right| \leq D^*_{N,\boldsymbol{\gamma},p}(\boldsymbol{z}) \left(\sum_{\mathrm{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathrm{u}}^{-q} \int_{[0,1]^{|\mathrm{u}|}} \left| \frac{\partial^{|\mathrm{u}|}}{\partial \boldsymbol{x}_{\mathrm{u}}} f(\boldsymbol{x}_{\mathrm{u}}, \mathbf{1}) \right|^q \mathrm{d}\boldsymbol{x}_{\mathrm{u}} \right)^{1/q}.$$

It is now obvious that the weighted discrepancy defined by (2.2) may be viewed as a L_∞ version of the weighted star discrepancy. Next, we see that we have

$$D^*_{N,\boldsymbol{\gamma},p}(\boldsymbol{z}) \leq \left(\sum_{\mathrm{u} \subseteq \mathcal{D}} \left(\boldsymbol{\gamma}_{\mathrm{u}} \sup_{\boldsymbol{x}_{\mathrm{u}} \in [0,1]^{|\mathrm{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathrm{u}}, \mathbf{1}), P_N)| \right)^p \right)^{1/p}.$$

Jensen's inequality as quoted in [13, Theorem 19, p. 28], states that if a_i are arbitrary non-negative numbers and $0 < t < s$, then

$$\left(\sum a_i^s \right)^{1/s} \leq \left(\sum a_i^t \right)^{1/t}.$$

Therefore, if we take $t = 1$ and $p = s \geq 1$, we have

$$\left(\sum a_i^p \right)^{1/p} \leq \sum a_i.$$

Since $p \geq 1$, by applying Jensen's inequality, we obtain

$$D^*_{N,\boldsymbol{\gamma},p}(\boldsymbol{z}) \leq \sum_{\mathrm{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathrm{u}} \sup_{\boldsymbol{x}_{\mathrm{u}} \in [0,1]^{|\mathrm{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathrm{u}}, \mathbf{1}), P_N)|.$$

The right-hand-side of this inequality is the weighted star discrepancy defined by (3.2) and analysed in this chapter. In conclusion, it will follow that under the assumption of summability for the weights, the generating vector $\boldsymbol{z}$ for an

intermediate-rank lattice rule may be constructed component-by-component so that the corresponding L_p weighted star discrepancy satisfies

$$D^*_{N,\boldsymbol{\gamma},p}(\boldsymbol{z}) = O(n^{-1+\delta}), \quad \forall \delta > 0,$$

with the involved constant independent of the dimension but depending on δ, ℓ, r and the weights.

Let us remark that in [35], the optimal rate of convergence $O(n^{-1+\delta})$ was achieved for the weighted L_2 discrepancy but for randomly shifted lattice rules of the form (1.6). The results in this chapter indicate that the CBC construction produces a pure deterministic point set for which the optimal rate of convergence can also be achieved for the weighted L_2 discrepancy.

We also mention that much of the earlier work on lattice rules (for instance [35], [36], [37], and [52]) has been developed by using a L_2 version of the discrepancy as a criterion of goodness. In all these papers, it was assumed that the weights are product. The conclusion that follows from the analysis developed in this section is that under a product weighted assumption, the results obtained here allow more generality since the bound on the weighted star discrepancy (3.2) allows subsequent bounds for L_p versions of the weighted star discrepancy for any $p \geq 1$, hence including bounds for the L_2 weighted star discrepancy.

Chapter 4

Korobov lattice rules based on the weighted star discrepancy

This chapter refines the results from Chapters 2 and 3 by studying the construction of Korobov lattice rules based on the weighted star discrepancy. If the weights are general, we establish the existence of good Korobov rank-1 lattice rule with a prime number of points. Then, under a product weighted assumption, we prove that there exists a Korobov-type generating vector that produces good intermediate-rank lattice rules. In both situations, we show that the resulting Korobov lattice rules are good in the sense of having a low weighted star discrepancy.

4.1 Introduction

In Chapters 2 and 3, we considered rank-1 lattice rules with general weights and intermediate-rank lattice rules with product weights. In this chapter, we refine the corresponding results from the previous chapters in the situation when the generating vector $\boldsymbol{z}$ has the so-called Korobov form, that is,

$$\boldsymbol{z}(a) := (1, a, \ldots, a^{d-1}) \,(\mathrm{mod}\, n),$$

where n is prime and a is a suitable integer chosen from $\mathcal{Z}_n = \{1, 2, \ldots, n-1\}$. This form of the generating vector was introduced in Chapter 1 by (1.8).

The usual weighted star discrepancy given by (2.2) and (3.2) will be used as a criterion of goodness. In the next section, we establish that under a general weighted setting, good Korobov rank-1 lattice rules do exist, while in Section 4.3, we consider intermediate-rank lattice rules with product weights and refine the results from Chapter 3 in the situation when the generating vector is of Korobov type.

Korobov lattice rules have been studied in [61], where the function spaces were either a weighted Korobov space of periodic functions or a weighted Sobolev space of non-periodic functions. Both function spaces were reproducing kernel Hilbert spaces, while the weights were assumed to be product. Here, we establish results for Korobov rank-1 lattice rules under a general weighted assumption and for Korobov intermediate-rank lattice rules with product weights.

We should also remark that Korobov lattice rules have some limitations. For instance, unlike lattice rules constructed using the CBC technique in the previous two chapters, Korobov lattice rules are not extensible in dimension. As an aside, it is interesting to mention that there are some limited results regarding extensible Korobov lattice rules in number of points. These results can be found in [12] and are based on a quality measure that looks at the two-dimensional projections.

As we shall also point out later, a fast construction analogous to the fast CBC construction seems unlikely for Korobov-lattice rules. Moreover, the bounds on the weighted star discrepancy are worse that the bounds for the corresponding lattice rules constructed using the CBC technique, but we still obtain tractability bounds on the weighted star discrepancy. Nevertheless, as we mentioned in the first chapter, Korobov lattice rules are important due to their historical significance (see [32] and [33] for further details) in the sense that Korobov lattice rules were the first known low discrepancy lattice rules. For completeness, we consider such Korobov lattice rules in this chapter.

4.2 Korobov rank-1 lattice rules with general weights

In this section, we assume that the weights are general and n is prime (same assumptions as in Chapter 2). Hence, we assume that for any non-empty subset $\mathfrak{u} \subseteq \mathcal{D}$, we have

$$\boldsymbol{\gamma}_{\mathfrak{u}} \le \boldsymbol{\gamma}_{\mathfrak{g}} \quad \text{for any} \quad \emptyset \ne \mathfrak{g} \subseteq \mathfrak{u}.$$

We consider now the weighted star discrepancy given by (2.2), that is,

$$D^*_{n,\boldsymbol{\gamma}} = \max_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{x}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} |\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)|,$$

where all the notations above are as in Chapter 2. This discrepancy was obtained in connection with Zaremba's identity and Hölder's inequality for integrals and sums (see (1.13)). If $\boldsymbol{z}$ is the generating vector of a rank-1 lattice rule, then it follows from Lemma 2.4 (see also [48, Lemma 1]) that

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}(a)) \le \frac{1}{n} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2} e^2_{n,d}(\boldsymbol{z}), \tag{4.1}$$

where

$$e^2_{n,d}(\boldsymbol{z}) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_n(\boldsymbol{z}, \mathfrak{u}),$$

with $\widetilde{R}_n(\boldsymbol{z}, \mathfrak{u})$ defined by (2.15) in Chapter 2. If $\boldsymbol{z}$ is a Korobov-type generating vector, then

$$\widetilde{R}_n(\boldsymbol{z}(a), \mathfrak{u}) := \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j(a)/n}}{|h|} \right),$$

where $z_j(a) = a^{j-1} \pmod n$. Also from Chapter 2 (see (2.17)), we know that $\widetilde{R}_n(\boldsymbol{z}(a), \mathfrak{u})$ can be expressed as

$$\widetilde{R}_n(\boldsymbol{z}(a), \mathfrak{u}) = \sum_{\substack{\boldsymbol{h} \in \widetilde{E}^*_{n,|\mathfrak{u}|} \\ \boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a) \equiv 0 \,(\bmod\, n)}} \prod_{j \in \mathfrak{u}} \frac{1}{|h_j|},$$

where we recall that (see also (2.16))

$$\widetilde{E}^*_{n,s} = \{\boldsymbol{h} \in \mathbb{Z}^s : -n/2 < h_j \le n/2,\ h_j \ne 0,\ 1 \le j \le s\}.$$

Further bounds on the weighted star discrepancy can be obtained by making use of (4.1). For the analysis carried out in this chapter, the following result from number theory is very useful (see [14]):

Theorem 4.1 *If n is prime and $g(x) = h_0 + h_1 x + \cdots + h_m x^m$ is a polynomial with integer coefficients, $D = \gcd(h_0, \ldots, h_m)$ and $\boldsymbol{h} = (h_0, h_1, \ldots, h_m)$, then the number $A_n(\boldsymbol{h})$ of integers x with $0 \le x \le n-1$ satisfying $g(x) \equiv 0 \pmod{n}$ is given by*

$$A_n(\boldsymbol{h}) \begin{cases} = n, & D \equiv 0 \,(\mathrm{mod}\, n), \\ \le m, & \text{otherwise.} \end{cases}$$

Next, we focus on the quantity $e^2_{n,d}(\boldsymbol{z}(a))$ with the generating vector $\boldsymbol{z}$ having the Korobov form (1.8). We can now prove the following result:

Theorem 4.2 *If n is prime, then there exists an $a \in \mathcal{Z}_n$ such that*

$$e^2_{n,d}(\boldsymbol{z}(a)) \le \frac{d-1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} S_n^{|\mathfrak{u}|}, \tag{4.2}$$

where S_n is as defined in Chapter 2, namely

$$S_n = \sum_{-n/2 < h \le n/2}{}' \frac{1}{|h|}.$$

Proof. We first define the mean of the quantities $e^2_{n,d}(\boldsymbol{z}(a))$ over all $a \in \mathcal{Z}_n$ by

$$M_{n,d,\boldsymbol{\gamma}} := \frac{1}{n-1} \sum_{a=1}^{n-1} e^2_{n,d}(\boldsymbol{z}(a)).$$

By making use of the expression for $e^2_{n,d}(\boldsymbol{z}(a))$, we next obtain:

$$\begin{aligned} M_{n,d,\boldsymbol{\gamma}} &= \frac{1}{n-1} \sum_{a=1}^{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} \widetilde{R}_n(\boldsymbol{z}(a), \mathfrak{u}) \\ &= \frac{1}{n-1} \sum_{a=1}^{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} \left(\sum_{\substack{\boldsymbol{h} \in \widetilde{E}^*_{n,|\mathfrak{u}|} \\ \boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a) \equiv 0 \,(\mathrm{mod}\, n)}} \prod_{j \in \mathfrak{u}} \frac{1}{|h_j|} \right) \\ &= \frac{1}{n-1} \sum_{a=1}^{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} \sum_{\boldsymbol{h} \in \widetilde{E}^*_{n,|\mathfrak{u}|}} \prod_{j \in \mathfrak{u}} \frac{1}{|h_j|} \delta_n(\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a)), \end{aligned}$$

where

$$\delta_n(m) = \begin{cases} 1, & m \equiv 0 \,(\mathrm{mod}\, n), \\ 0, & \text{otherwise.} \end{cases} \tag{4.3}$$

Then the mean can be written as

$$M_{n,d,\boldsymbol{\gamma}} = \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{\boldsymbol{h} \in \widetilde{E}^*_{n,|\mathfrak{u}|}} \prod_{j \in \mathfrak{u}} \frac{1}{|h_j|} \left(\sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a)) \right). \tag{4.4}$$

We see that the last sum in (4.4) represents the number of solutions of the congruency $\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a) \equiv 0 \,(\mathrm{mod}\, n)$. Since n is prime and $\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a)$ is a polynomial of degree at most $d-1$ in a with coefficients that are not multiples of n, it follows from Theorem 4.1 that

$$\sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a)) \leq d - 1.$$

Replacing this in (4.4), we obtain

$$M_{n,d,\boldsymbol{\gamma}} \leq \frac{d-1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{\boldsymbol{h} \in \widetilde{E}^*_{n,|\mathfrak{u}|}} \prod_{j \in \mathfrak{u}} \frac{1}{|h_j|} = \frac{d-1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}. \tag{4.5}$$

Clearly, there must be an $a \in \mathcal{Z}_n$ such that

$$e^2_{n,d}(\boldsymbol{z}(a)) \leq M_{n,d,\boldsymbol{\gamma}},$$

which together with (4.5), leads to the desired result. □

Subsequent results can be obtained for order-dependent and finite-order weights, which were introduced by Definition 2.2 and Definition 2.3 in Chapter 2.

Recall that order-dependent weights are those whose dependence on $\mathfrak{u}$ is only through the cardinality of $\mathfrak{u}$. Assuming that sets having the same cardinality have equal values of the associated weights, we can use just d weights, say $\Gamma_1, \Gamma_2, \ldots, \Gamma_d$, where Γ_ℓ denotes the weight associated with any set containing ℓ elements for $1 \leq \ell \leq d$. The next result follows directly from Theorem 4.2 by taking $\boldsymbol{\gamma}_{\mathfrak{u}} = \Gamma_\ell$ whenever $|\mathfrak{u}| = \ell$ and noting that the number of subsets of $\mathcal{D}$ with cardinality ℓ is $\binom{d}{\ell}$.

Corollary 4.3 *Let n be prime and suppose the weights are order-dependent. Then there exists an $a \in \mathcal{Z}_n$ such that the Korobov-type generating vector $\boldsymbol{z}(a)$ satisfies*

$$e^2_{n,d}(\boldsymbol{z}(a)) \leq \frac{d-1}{n-1} \sum_{\ell=1}^{d} \Gamma_\ell \binom{d}{\ell} S_n^\ell.$$

Next, let's assume that the weights are finite-order. This means that there exists a positive integer q such that $\boldsymbol{\gamma}_{\mathfrak{u}} = 0$ for all $\mathfrak{u}$ with $|\mathfrak{u}| > q$. We shall take q^* to be the smallest integer satisfying this condition. We then obtain the following result:

Corollary 4.4 *Let n be prime and suppose the weights are finite-order. Then there exists an $a \in \mathcal{Z}_n$ such that the Korobov-type generating vector $\boldsymbol{z}(a)$ satisfies*

$$e^2_{n,d}(\boldsymbol{z}(a)) \leq \frac{d-1}{n-1} \sum_{\substack{\mathfrak{u} \subseteq \mathcal{D} \\ 1 \leq |\mathfrak{u}| \leq q^*}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}.$$

We can combine these two classes of weights to consider the situation when the weights are both order-dependent and finite-order.

Corollary 4.5 *Let n be prime and suppose the weights are both order-dependent and finite-order. Then there exists a Korobov-type generating vector $\boldsymbol{z}(a)$ such that*

$$e^2_{n,d}(\boldsymbol{z}(a)) \leq \frac{d-1}{n-1} \sum_{\ell=1}^{q^*} \Gamma_\ell \binom{d}{\ell} S_n^\ell.$$

4.2.1 Tractability results

First, let us remark that from (4.1) and (4.2), it will follow that there exists a Korobov-type generating vector $\boldsymbol{z}(a)$ such that the weighted star discrepancy satisfies the following bound:

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}(a)) \leq \frac{1}{n} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{d-1}{2(n-1)} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|}. \tag{4.6}$$

Since $S_n = O(\ln n)$ (see (2.24)), it will follow from (4.6) that the weighted star discrepancy has order of magnitude of $O(n^{-1}(\ln n)^d)$ with the implied constant depending only on d. As mentioned also in the previous chapters,

such a convergence rate attained by the star discrepancy is considered to be the best possible in an unweighted setting and thus, we should consider such a bound as being "good". However, under appropriate conditions over the weights we can obtain tractability and strong tractability results.

Theorem 4.6 *If $n \geq 3$ is prime with the weights chosen such that $\boldsymbol{\gamma}_{\mathfrak{u}} \leq \boldsymbol{\gamma}_{\mathfrak{g}}$ for any $\emptyset \neq \mathfrak{g} \subseteq \mathfrak{u}$ and*

$$\sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \leq C(\boldsymbol{\gamma}, \delta) n^{\delta}, \tag{4.7}$$

for some $\delta > 0$, where $C(\boldsymbol{\gamma}, \delta)$ is independent of d and n, then there exists a Korobov-type generating vector $\boldsymbol{z}(a)$ such that the corresponding weighted star discrepancy satisfies the error bound

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}(a)) = O(dn^{-1+\delta}), \quad \textit{for any} \quad \delta > 0,$$

where the implied constant depends only on the weights.

Proof. Let us remark first that from (4.6) and the condition (4.7), we obtain

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{1}{n} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{(d-1) C(\boldsymbol{\gamma}, \delta) n^{\delta}}{2(n-1)}.$$

From the proof of Theorem 2.16, we have

$$\max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} \leq \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \leq C(\boldsymbol{\gamma}, \delta) n^{\delta}.$$

Consequently, this leads to

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \frac{C(\boldsymbol{\gamma}, \delta) n^{\delta}}{n} + \frac{(d-1) C(\boldsymbol{\gamma}, \delta) n^{\delta}}{2(n-1)} \leq d C(\boldsymbol{\gamma}, \delta) n^{-1+\delta},$$

which shows that the dependency of the bound on d is at most linear, and hence we obtain the desired result. □

Let us remark that the condition (4.7) is a sufficient condition of tractability. If the weights satisfy the stronger condition

$$(d-1) \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_n^{|\mathfrak{u}|} \leq C(\boldsymbol{\gamma}, \delta) n^{\delta},$$

for some $\delta > 0$, where $C(\boldsymbol{\gamma}, \delta)$ is independent of d and n, then such a condition will ensure strong tractability. As an aside, we remark that this strong tractability condition involves a dependence of the weights on the dimension. Such weights depending on the dimension have been also considered in [9].

4.3 Korobov intermediate-rank lattice rules

In this section, we refine the results from Chapter 3 for intermediate-rank lattice rules when the generating vector $\boldsymbol{z}$ is of the Korobov form (1.8). Thus, we recall that n is assumed to be prime, $\ell \geq 1$ is an integer satisfying $\gcd(\ell, n) = 1, r$ is a fixed integer taken from the set $\{0, 1, \ldots, d\}$ and $N = \ell^r n$. The intermediate-rank lattice rules considered here are of the form (see also (1.7))

$$Q^{(r)}_{N,d}(f) = \frac{1}{\ell^r n} \sum_{m_r=0}^{\ell-1} \cdots \sum_{m_1=0}^{\ell-1} \sum_{k=0}^{n-1} f\left(\left\{\frac{k\boldsymbol{z}}{n} + \frac{(m_1, \ldots, m_r, 0, \ldots, 0)}{\ell}\right\}\right).$$

If P_N denotes the points of this lattice rule, then it will follow that the weighted star discrepancy of this point set satisfies (see (3.5))

$$D^*_{N,\boldsymbol{\gamma}}(P_N) \leq \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1 - (1 - 1/N)^{|\mathfrak{u}|}\right) + \frac{1}{2} e^2_{N,d}(\boldsymbol{z}(a)), \tag{4.8}$$

where $e^2_{N,d}(\boldsymbol{z}(a))$ is as given by (3.8), while the weights are assumed to be product. Since $\boldsymbol{z}$ is a Korobov type vector, then $z_j = a^{j-1} \pmod n$ for every $1 \leq j \leq d$. Let us also introduce

$$\hat{h}_j = \begin{cases} \ell h_j, & \text{if } 1 \leq j \leq r \text{ and } h_j \neq 0, \\ h_j, & \text{if } r+1 \leq j \leq d \text{ and } h_j \neq 0, \\ 1, & \text{if } h_j = 0. \end{cases}$$

In Chapter 3, we have established that

$$e^2_{N,d}(\boldsymbol{z}(a)) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} R_N(\boldsymbol{z}(a), \mathfrak{u}), \tag{4.9}$$

where it follows from (3.8) that

$$R_N(\boldsymbol{z}(a), \mathfrak{u}) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(1 + {\sum_{-\tilde{N}_j/2 < h_j \leq \tilde{N}_j/2}}' \frac{e^{2\pi \mathrm{i} h_j k \hat{z}_j(a)/n}}{|\hat{h}_j|}\right) - 1.$$

Recall that $\tilde{N}_j$ and $\hat{z}_j$ are given by (see also (3.10) and (3.11)):

$$\tilde{N}_j = \begin{cases} N/\ell = \ell^{r-1} n, & 1 \leq j \leq r, \\ N, & r+1 \leq j \leq d, \end{cases}$$

and

$$\hat{z}_j = \begin{cases} \ell z_j, & 1 \le j \le r, \\ z_j, & r+1 \le j \le d. \end{cases}$$

Lemma 3.1 leads to

$$\sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} \left(1 - (1 - 1/N)^{|\mathfrak{u}|}\right) = O(n^{-1}), \tag{4.10}$$

where the implied constant depends on ℓ, r and the weights. Next, we focus on the quantity $e^2_{N,d}(\boldsymbol{z})$ given by (4.9). Let us denote

$$\mathcal{E}_{\mathfrak{u}} := \{\boldsymbol{h} \in \mathbb{Z}^{|\mathfrak{u}|} : -\tilde{N}_j/2 < h_j \le \tilde{N}_j/2,\ j \in \mathfrak{u}\},$$

with $\mathcal{E}^*_{\mathfrak{u}} = \mathcal{E}_{\mathfrak{u}} - \{\mathbf{0}\}$. Consider now

$$\begin{aligned} R_N(\boldsymbol{z}(a)), \mathfrak{u}) &= \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(1 + {\sum_{-\tilde{N}_j/2 < h_j \le \tilde{N}_j/2}}' \frac{e^{2\pi \mathrm{i} h_j k \hat{z}_j(a)/n}}{|\hat{h}_j|}\right) - 1 \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-\frac{\tilde{N}_j}{2} < h_j \le \frac{\tilde{N}_j}{2}} \frac{e^{2\pi \mathrm{i} h_j k \hat{z}_j(a)/n}}{|\hat{h}_j|}\right) - 1 \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\boldsymbol{h} \in \mathcal{E}_{\mathfrak{u}}} \frac{\left(e^{2\pi \mathrm{i} \boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a)/n}\right)^k}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|} - 1 \\ &= \sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \frac{1}{n} \sum_{k=0}^{n-1} \frac{\left(e^{2\pi \mathrm{i} \boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a)/n}\right)^k}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|} \\ &= \sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \frac{\delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a))}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|}, \end{aligned}$$

where $\delta_n(m)$ was defined in the previous section by (4.3). Using this in (4.9), we obtain

$$e^2_{N,d}(\boldsymbol{z}(a)) = \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \in \mathfrak{u}} \gamma_j\right) \sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \frac{\delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a))}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|}. \tag{4.11}$$

Next, by defining a mean over all quantities $e^2_{N,d}(\boldsymbol{z}(a))$, we prove the existence of a good Korobov-type generating vector.

Theorem 4.7 *Let n be prime and $e^2_{N,d}(\boldsymbol{z}(a))$ be defined by* (4.9)*. Then, there exists an $a \in \mathcal{Z}_n$ such that*

$$e^2_{N,d}(\boldsymbol{z}(a)) \le \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j/n}\right) + \frac{d-1}{n-1} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) - \frac{nd-1}{n(n-1)} \prod_{j=1}^{d} \beta_j, \tag{4.12}$$

where $\beta_j = 1 + \gamma_j$*, while* $\tilde{\gamma}_j$ *are defined by (see also* (3.9)*):*

$$\tilde{\gamma}_j = \begin{cases} \gamma_j/\ell, & 1 \leq j \leq r, \\ \gamma_j, & r+1 \leq j \leq d. \end{cases}$$

Proof. As in the previous section, the mean over all quantities $e^2_{N,d}(\boldsymbol{z}(a))$ is given by

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{n-1} \sum_{a=1}^{n-1} e^2_{N,d}(\boldsymbol{z}(a)).$$

Using now (4.11), we obtain

$$\begin{aligned} M_{N,d,\boldsymbol{\gamma}} &= \frac{1}{n-1} \sum_{a=1}^{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \in \mathfrak{u}} \gamma_j \right) \sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \frac{\delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a))}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|} \\ &= \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \in \mathfrak{u}} \gamma_j \right) \left(\sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \frac{1}{\prod_{j \in \mathfrak{u}} |\hat{h}_j|} \cdot \frac{1}{n-1} \sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a)) \right) \\ &= \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left(\prod_{j \in \mathfrak{u}} \gamma_j \right) (\sigma_1 + \sigma_2), \end{aligned} \tag{4.13}$$

where σ_1 denotes the expression in the inner brackets obtained when $\boldsymbol{h}$ has all the components a multiple of n, while σ_2 denotes the same expression obtained when at least one component of $\boldsymbol{h}$ is not a multiple of n. Let's remark that a similar decomposition has been used in [61]. When all the components of $\boldsymbol{h}$ are multiples of n, we first observe that

$$\frac{1}{n-1} \sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a)) = 1,$$

and hence we can write σ_1 as

$$\sigma_1 = \sum_{\boldsymbol{h} \in \mathcal{E}^*_{\mathfrak{u}}} \prod_{j \in \mathfrak{u}} \frac{1}{|\hat{h}_j|} = \sum_{\boldsymbol{h} \in \mathcal{E}_{\mathfrak{u}}} \prod_{j \in \mathfrak{u}} \frac{1}{|\hat{h}_j|} - 1 = \prod_{j \in \mathfrak{u}} \left(1 + {\sum_{-\frac{\tilde{N}_j}{2} < h_j \leq \frac{\tilde{N}_j}{2}}}' \frac{1}{|\hat{h}_j|} \right) - 1.$$

Since all the components of $\boldsymbol{h}$ are multiples of n, we may write $h_j = n m_j$ and we obtain that $-\frac{\tilde{N}_j}{2} < h_j \leq \frac{\tilde{N}_j}{2}$ is equivalent to $-\frac{\tilde{N}_j/n}{2} < m_j \leq \frac{\tilde{N}_j/n}{2}$. This leads to

$$\sigma_1 \leq \frac{1}{n} \left[\prod_{\substack{1 \leq j \leq r \\ j \in \mathfrak{u}}} \left(1 + \frac{S_{\tilde{N}_j/n}}{\ell} \right) \prod_{\substack{r+1 \leq j \leq d \\ j \in \mathfrak{u}}} \left(1 + S_{\tilde{N}_j/n} \right) - 1 \right]. \tag{4.14}$$

Let us remark that $\tilde{N}_j/n$ takes either the value ℓ^{r-1} or ℓ^r, which indicates that $\sigma_1 = O(n^{-1})$. Next, in order to evaluate σ_2, we first observe that the sum $\sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a))$ in (4.13) represents the number of solutions of the congruency $\boldsymbol{h} \cdot \boldsymbol{z}_{\mathfrak{u}}(a) \equiv 0 \,(\mathrm{mod}\, n)$. Since n is prime and $\boldsymbol{h}$ has at least one component which is not a multiple of n, then $\gcd\{h_j : j \in \mathfrak{u}\}$ cannot be a multiple of n. Using Theorem 4.1, it follows that

$$\sum_{a=1}^{n-1} \delta_n(\boldsymbol{h} \cdot \hat{\boldsymbol{z}}_{\mathfrak{u}}(a)) \leq d - 1,$$

which leads to

$$\sigma_2 \leq \frac{d-1}{n-1} \left[\prod_{\substack{1 \leq j \leq r \\ j \in \mathfrak{u}}} \left(1 + \frac{S_{\tilde{N}_j}}{\ell}\right) \prod_{\substack{r+1 \leq j \leq d \\ j \in \mathfrak{u}}} \left(1 + S_{\tilde{N}_j}\right) - 1 \right]. \tag{4.15}$$

Now, from (4.13), (4.14) and (4.15), we obtain:

$$\begin{aligned} M_{N,d,\boldsymbol{\gamma}} \;\leq\; & \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left[\prod_{j \in \mathfrak{u}} \left(\gamma_j + \tilde{\gamma}_j S_{\tilde{N}_j/n}\right) - \prod_{j \in \mathfrak{u}} \gamma_j \right] \\ & + \frac{d-1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \left[\prod_{j \in \mathfrak{u}} \left(\gamma_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) - \prod_{j \in \mathfrak{u}} \gamma_j \right] \\ = \;& \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j/n}\right) - \frac{1}{n} \prod_{j=1}^{d} \beta_j \\ & + \frac{d-1}{n-1} \left[\prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right) - \prod_{j=1}^{d} \beta_j \right], \end{aligned}$$

which simplifies to (4.12). Clearly, there must be an $a \in \mathcal{Z}_n$ such that

$$e^2_{N,d}(\boldsymbol{z}(a)) \leq M_{N,d,\boldsymbol{\gamma}},$$

which together with the previous inequality, leads to the desired result. □

4.3.1 Tractability results

The bound given by (4.12), together with (4.8) and (4.10) suggest that the weighted star discrepancy has order of magnitude of $O(n^{-1}(\ln n)^d))$ with the involved constant depending on d, ℓ and r. Let us recall from Chapter 3 that under a condition of summability for the weights, strong tractability followed

for intermediate-rank lattice rules constructed using the CBC technique. For Korobov intermediate-rank lattice rules, we can prove the following result:

Theorem 4.8 *If $n \geq 3$ and the weights are summable, that is, $\sum_{j=1}^{\infty} \gamma_j < \infty$, then there exists a Korobov-type generating vector $\boldsymbol{z}(a)$ such that the weighted star discrepancy has the order of magnitude of $O(dn^{-1+\delta})$, where the involved constant depends only on ℓ, r and the weights.*

Proof. We see first that the right-hand-side of (4.12) can be further bounded, so that we can write

$$e^2_{N,d}(\boldsymbol{z}(a)) \leq \frac{1}{n} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j/n}\right) + \frac{d-1}{n-1} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j}\right). \tag{4.16}$$

From (2.24), it follows that $S_{\tilde{N}_j} \leq 2 \ln \tilde{N}_j = O(\ln n)$ for every $1 \leq j \leq d$, with the involved constant depending on ℓ and r. Let's observe first that since $\tilde{N}_j/n$ is independent of n, we can write $\beta_j + \tilde{\gamma}_j S_{\tilde{N}_j/n} \leq 1 + \alpha\gamma_j$ where $\alpha > 1$ is a constant. Since the weights γ_j are summable, we see that the first term from the right-hand-side of (4.16) can be bounded as follows:

$$\frac{1}{n} \prod_{j=1}^{d} (1 + \alpha\gamma_j) \leq \frac{1}{n} e^{\sum_{j=1}^{d} \ln(1+\alpha\gamma_j)} \leq \frac{1}{n} \exp\left(\alpha \sum_{j=1}^{\infty} \gamma_j\right) = O(n^{-1}),$$

where the involved constant depends on ℓ, r and the weights but is independent of d and n. Using Theorem 3.4, we see that the second term on the right-hand-side of (4.16) can be further bounded by $dC(\boldsymbol{\gamma}, \delta, \ell, r)\, n^{\delta} \prod_{j=1}^{\infty} \beta_j$. It will follow that the weighted star discrepancy achieves the error bound of $O(dn^{-1+\delta})$ for any $\delta > 0$ and with the involved constant depending only on ℓ, r and the weights. Since the dependency on d is at most linear, the summability of the weights ensures tractability of the integration problem. □

4.4 The construction algorithm

As mentioned in the first section of this chapter, the Korobov lattice rules constructed here are not extensible in dimension. The construction algorithm can be described as follows:

Construction algorithm for Korobov lattice rules

For $a \in \mathcal{Z}_n$ do:

Select a such that $e^2_{N,d}(\boldsymbol{z}(a))$ is minimised.

For the rank-1 lattice rules considered in Section (4.2), let's recall first that $N = n$ and

$$e^2_{N,d}(\boldsymbol{z}(a)) = \sum_{\mathrm{u} \subseteq \mathcal{D}} \gamma_{\mathrm{u}} \left(\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathrm{u}} \left(\sum_{-n/2 < h \le n/2}{}' \frac{e^{2\pi \mathrm{i} h k a^{j-1}/n}}{|h|} \right) \right).$$

It will follow from Chapter 2 that the total complexity of the algorithm will be $O(n^2 d\tau)$, where τ is the total number of non-zero weights plus $O(n)$ storage for the values of the inner sum. Full details of the analysis of the computational cost of the algorithm may be found in [48] and in Chapter 2. For finite-order weights, the cost of the construction is $O(n^2 d^{q^*+1})$, while for order-dependent weights the cost is $O(n^2 d^2)$.

For the intermediate-rank lattice rules considered in the previous section, let us recall that

$$e^2_{N,d}(\boldsymbol{z}(a)) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(\beta_j + \tilde{\gamma}_j \sum_{-\frac{\tilde{N}_j}{2} < h \le \frac{\tilde{N}_j}{2}}{}' \frac{e^{2\pi \mathrm{i} h k \hat{z}_j(a)/n}}{|h|} \right) - \prod_{j=1}^{d} \beta_j.$$

It will follow from Chapter 3 that the cost of the algorithm will be $O(n^2 d)$ plus $O(n)$ for storage.

Finally, let us remark that in [44] a fast algorithm for constructing lattice rules was proposed. In general terms, the fast construction replaced the n^2 factor occurring in the evaluation of the cost by a much smaller factor of $n \ln n$. This fast algorithm was applicable for lattice rules for which the generating vector was constructed using a component-by-component technique. At this stage however, it does not seem clear that such an algorithm could also be used for Korobov-type lattice rules.

Chapter 5

Good rank-1 lattice rules with a composite number of points based on the product weighted star discrepancy

Rank-1 lattice rules based on a weighted star discrepancy with weights of a product form have been constructed in numerous research papers under the assumption that the number of points is prime. For general weights, a construction of rank-1 lattice rules was presented in Chapter 2 also under the assumption that n is prime. In the non-prime case however, there aren't too many known results to date mainly due to the technical difficulties that arise. Nevertheless, in this chapter we fill this gap and extend previous results obtained in [29] to the non-prime case. We show that if the weights are summable, there exist lattice rules whose weighted star discrepancy is $O(n^{-1+\delta})$, for any $\delta > 0$, with the implied constant independent of the dimension, but dependent on δ and the weights. Then we show that the generating vector of such a lattice rule can be constructed using the component-by-component (CBC) technique and, in the final part of the chapter, we analyse the cost of the CBC construction. The results from this chapter are based on the paper [50].

5.1 Introduction

In order to approximate integrals over the d-dimensional unit cube, in this chapter we consider rank-1 lattice rules of the form (see also (1.5))

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

where as usual, $\boldsymbol{z} \in \mathbb{Z}^d$ denotes the generating vector of these lattice rules and all the components of $\boldsymbol{z}$ are assumed to be relatively prime with n.

In this paper we extend the results in [29] by constructing rank-1 lattice rules with a composite number of points. Hence, the same assumptions as in [29] will be used here with the main difference that n is assumed to be just a positive integer. In the vast majority of earlier research papers as well as in the previous chapters, it was assumed that n was prime; an assumption which simplifies the analysis of the problem.

However there are some known results in the non-prime case. For instance, it has been proved in [10], [41], or [42, Chapter 5] that good lattice rules with a non-prime number of points do exist. Several measures of goodness were used in those works, but under the assumptions that variables are equally important. In this chapter however, we will employ a weighted star discrepancy as a criterion of goodness.

A constructive approach in the non-prime case has been proposed in [36], where the integrands were assumed to belong to certain reproducing kernel Hilbert spaces such as weighted Korobov spaces of periodic functions or weighted Sobolev spaces with square-integrable mixed first derivatives. Here we require the integrands to have the weaker requirement of integrable mixed first derivatives. Let us remark that in [35] it was proved that in the reproducing kernel Hilbert spaces of [36], the component-by-component construction (used also here) achieves the optimal rate of convergence $O(n^{-1+\delta})$, for any $\delta > 0$. In [7], the results in [35] were extended to the non-prime case.

Let us also mention that lattice rules with a composite number of points have become of more interest since the introduction of extensible lattice rules

in [18]. Later, extensible lattice rules have been studied in [19] and [20]. In [20], it was shown that extensible lattice rules in number of points with a low weighted star discrepancy do exist, but the proof was non-constructive. More recently, in [8], a possible way of constructing extensible lattice rules was proposed. Therein, it was assumed that n is of the particular form p^m with $p \geq 2$ an arbitrary prime and it has been shown that lattice rules extensible in number of points based on the weighted star discrepancy can be constructed, but the results were not generalised to arbitrary integers.

As mentioned earlier, throughout this chapter we make similar assumptions over the weights as in [29]. Let $\mathfrak{u}$ be an arbitrary non-empty subset of $\mathcal{D} = \{1, 2, \ldots, d-1, d\}$ and let us introduce a sequence of positive weights $\{\gamma_j\}_{j=1}^{\infty}$, which describe the decreasing importance of the successive coordinates x_j. As usual, $\boldsymbol{\gamma}_{\mathfrak{u}}$ will be the weight associated with the set $\mathfrak{u}$ and, in this chapter, we assume that the weights $\{\boldsymbol{\gamma}_{\mathfrak{u}}\}$ are product. Hence $\boldsymbol{\gamma}_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ for every subset $\mathfrak{u} \subseteq \mathcal{D}$.

5.2 Bounds on the weighted star discrepancy

In this chapter, we consider a similar weighted star discrepancy as the one defined by (3.2), namely

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) := \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{x}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} \left| \mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n) \right|, \tag{5.1}$$

where $P_n = \{\{k\boldsymbol{z}/n\},\ 0 \leq k \leq n-1\}$. Such a weighted star discrepancy has arisen in Chapter 3 from the inequality (3.1). From Theorem 2.3 (see also (3.5)), it follows that the weighted star discrepancy given by (5.1) satisfies the inequality

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1 - (1 - 1/n)^{|\mathfrak{u}|} + \frac{R_n(\boldsymbol{z}, \mathfrak{u})}{2} \right), \tag{5.2}$$

where $R_n(\boldsymbol{z}, \mathfrak{u})$ is as given by (2.9), that is

$$R_n(\boldsymbol{z}, \mathfrak{u}) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(1 + \sum_{-n/2 < h \leq n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right) - 1.$$

To obtain bounds on $D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z})$, we see from (5.2) that we need to bound the quantity

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1-(1-1/n)^{|\mathfrak{u}|}\right)$$

and the quantity

$$e^2_{n,d}(\boldsymbol{z}) := \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} R_n(\boldsymbol{z},\mathfrak{u}). \tag{5.3}$$

Under the assumption that the weights are summable, that is, $\sum_{j=1}^{\infty}\gamma_j<\infty$, it follows from Lemma 3.1 that

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(1-(1-1/n)^{|\mathfrak{u}|}\right) = O(n^{-1}), \tag{5.4}$$

with the implied constant depending on the weights, but independent of d and n.

We now consider $e^2_{n,d}(\boldsymbol{z})$ in more detail and by expanding (5.3) in the same way as in Chapter 3 (see also [29]), we obtain

$$e^2_{n,d}(\boldsymbol{z}) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}(\beta_j+\gamma_j C_k(z_j)) - \prod_{j=1}^{d}\beta_j, \tag{5.5}$$

where we recall that $\beta_j = 1+\gamma_j$ for any $1\le j\le d$, and

$$C_k(z) = \sum_{-n/2<h\le n/2}{}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|}.$$

We can obtain a bound on $e^2_{n,d}(\boldsymbol{z})$ by obtaining a bound on a certain mean value of $e^2_{n,d}(\boldsymbol{z})$. The mean $M_{n,d,\boldsymbol{\gamma}}$ is defined by

$$M_{n,d,\boldsymbol{\gamma}} := \frac{1}{(\varphi(n))^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d} e^2_{n,d}(\boldsymbol{z}),$$

where φ is Euler's totient function and

$$\mathcal{Z}_n = \{z : z\in\{1,2,\ldots,n-1\},\ (z,n)=1\}.$$

In order to simplify some notations, throughout this chapter we shall use (z,n) to denote $\gcd(z,n)$. A bound on the mean $M_{n,d,\boldsymbol{\gamma}}$ is given next.

Theorem 5.1 *Let $n\ge 2$ be an integer and let us recall that*

$$S_n = \sum_{-n/2<h\le n/2}{}' \frac{1}{|h|}.$$

If the weights $\{\gamma_j\}_{j=1}^{\infty}$ *are summable, then*

$$M_{n,d,\boldsymbol{\gamma}} \leq \frac{1}{n}\prod_{j=1}^{d}(\beta_j+\gamma_j S_n)+O\left(\frac{\ln\ln(n+1)}{n}\right),$$

where the implied constant depends on the weights, but is independent of the dimension.

Proof. From the definition of the mean and (5.5), we have

$$\begin{aligned} M_{n,d,\boldsymbol{\gamma}} &= \frac{1}{(\varphi(n))^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d}\left(\frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}(\beta_j+\gamma_j C_k(z_j))-\prod_{j=1}^{d}\beta_j\right) \\ &= \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\frac{1}{\varphi(n)}\sum_{z_j\in\mathcal{Z}_n}(\beta_j+\gamma_j C_k(z_j))\right)-\prod_{j=1}^{d}\beta_j \\ &= \frac{1}{n}\prod_{j=1}^{d}(\beta_j+\gamma_j S_n)+\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{\varphi(n)}\sum_{z_j\in\mathcal{Z}_n}C_k(z_j)\right)-\prod_{j=1}^{d}\beta_j, \end{aligned}$$

where in the last step the $k=0$ term has been separated out and we have used the fact that $C_0(z)=S_n$. Let us denote

$$T_n(k)=\sum_{z\in\mathcal{Z}_n}C_k(z)=\sum_{z\in\mathcal{Z}_n}{\sum_{-n/2<h\leq n/2}}'\frac{e^{2\pi \mathrm{i}hkz/n}}{|h|}. \tag{5.6}$$

In fact this quantity has also been introduced in Chapter 2, but under the assumption that n was prime. In such a case it followed from Lemma 2.5 that $T_n(k)=-S_n$ for any $1\leq k\leq n-1$. The fact that the value of $T_n(k)$ is independent of k in the prime case allows a considerable simplification of the whole analysis. However here, since n is not necessarily prime, we need to employ asymptotic expansion techniques in order to evaluate (5.6). Going back to the mean, we see now that it can be written as

$$M_{n,d,\boldsymbol{\gamma}}=\frac{1}{n}\prod_{j=1}^{d}(\beta_j+\gamma_j S_n)+L_{n,d,\boldsymbol{\gamma}}-\prod_{j=1}^{d}\beta_j, \tag{5.7}$$

where

$$L_{n,d,\boldsymbol{\gamma}}=\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j+\frac{\gamma_j}{\varphi(n)}T_n(k)\right). \tag{5.8}$$

The rest of this proof follows many of the arguments used in the proof of [42, Theorem 5.10] (see also [10]). First, it may be shown that

$$T_n(k)=\sum_{a|n}\mu(a)\left(\frac{n}{a},k\right)S_{a(\frac{n}{a},k)}=\sum_{a|n}\mu\left(\frac{n}{a}\right)(a,k)\,S_{\frac{n(a,k)}{a}}, \tag{5.9}$$

where μ denotes the well-known Möbius function from number theory (see for instance [1]). If n is prime, then, as mentioned earlier, we obtain $T_n(k) = -S_n$ for any $1 \leq k \leq n-1$, which leads to the results obtained in [29]. From Lemma 2.9, we know that

$$S_m = 2\ln\ m + 2\omega - \ln 4 + \varepsilon\,(m)\,,$$

where ω is the Euler-Mascheroni constant, while $|\varepsilon(m)| < 4m^{-2}$. Using (5.9), we now obtain

$$T_n(k) = (2\ln n + 2\omega - \ln 4)B_n(k) - 2H_n(k) + V_n(k), \tag{5.10}$$

where

$$B_n(k) = \sum_{a|n} \mu\left(\frac{n}{a}\right)(a,k),$$

$$H_n(k) = \sum_{a|n} \mu\left(\frac{n}{a}\right)(a,k)\ln\frac{a}{(a,k)},$$

and

$$V_n(k) = \sum_{a|n} \mu\left(\frac{n}{a}\right)(a,k)\varepsilon\left(\frac{n(a,k)}{a}\right). \tag{5.11}$$

From the proof of [42, Theorem 5.10], we have $B_n(k) = 0$ for any $1 \leq k \leq n-1$. Using this result in (5.10), we get

$$T_n(k) = -2H_n(k) + V_n(k). \tag{5.12}$$

By combining (5.8) with (5.12), we obtain

$$L_{n,d,\boldsymbol{\gamma}} = \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j\left(-2J_n(k) + \frac{V_n(k)}{\varphi(n)}\right)\right), \tag{5.13}$$

where

$$J_n(k) = \frac{H_n(k)}{\varphi(n)}.$$

The proof of Theorem 5.10 in [42] yields $V_n(k) = O(1)$ with an absolute implied constant. Hence we have $V_n(k)/\varphi(n) = O(1/\varphi(n))$. This result together with (5.13) and $\beta_j = 1 + \gamma_j$ leads us to

$$L_{n,d,\boldsymbol{\gamma}} = \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(1 + \gamma_j(1 - 2J_n(k)) + \gamma_j O\left(\frac{1}{\varphi(n)}\right)\right). \tag{5.14}$$

Let us consider a prime p and denote by $e_p(n)$ the largest exponent such that $p^{e_p(n)}$ divides n. Then, also from the proof of [42, Theorem 5.10], we obtain

$$H_n(k) = \begin{cases} p^{e_p(k)}\varphi(n/p^{e_p(n)})\ln p, & \text{if } p \text{ is the unique prime with } e_p(n) > e_p(k), \\ 0, & \text{otherwise.} \end{cases}$$

If such a p exists, then by the definition of $e_p(n)$, we have $n/p^{e_p(n)}$ relatively prime with $p^{e_p(n)}$ and hence $\varphi(n/p^{e_p(n)})\varphi(p^{e_p(n)}) = \varphi(n)$. We then obtain

$$J_n(k) = \frac{p^{e_p(k)}\varphi(n/p^{e_p(n)})\ln p}{\varphi(n)} = \frac{p^{e_p(k)}\ln p}{\varphi(p^{e_p(n)})} = \frac{\ln p}{p^{\alpha_k}\,(p-1)},$$

where we put $\alpha_k = e_p(n) - e_p(k) - 1$, for $1 \le k \le n-1$. For each $1 \le k \le n-1$, it is not difficult to check that $-1 < 1 - 2\ln(p)/(p^{\alpha_k}(p-1)) < 1$ for any prime $p \ge 2$ and for any $\alpha_k \ge 0$. Hence, $1 + \gamma_j(1 - 2J_n(k)) \le 1 + \gamma_j = \beta_j$ for any $1 \le j \le d$. Considering now the product from (5.14), we obtain

$$\begin{aligned} & \prod_{j=1}^{d}\left(1 + \gamma_j(1 - 2J_n(k)) + \gamma_j O\left(\frac{1}{\varphi(n)}\right)\right) \\ \le\ & \prod_{j=1}^{d}\left(\beta_j + \gamma_j O\left(\frac{1}{\varphi(n)}\right)\right) \\ =\ & \prod_{j=1}^{d}\beta_j + \sum_{\mathfrak{u}\subseteq\mathcal{D}}\left(O\left(\frac{1}{\varphi(n)}\right)\right)^{|\mathfrak{u}|}\prod_{j\in\mathfrak{u}}\gamma_j\prod_{j\notin\mathfrak{u}}\beta_j \\ =\ & \prod_{j=1}^{d}\beta_j + O\left(\frac{1}{\varphi(n)}\right), \end{aligned} \tag{5.15}$$

where the implied constant depends on the quantity

$$\sum_{\mathfrak{u}\subseteq\mathcal{D}}\prod_{j\in\mathfrak{u}}\gamma_j\prod_{j\notin\mathfrak{u}}\beta_j \le \prod_{j=1}^{d}(\beta_j + \gamma_j).$$

Next, let us consider

$$\prod_{j=1}^{d}(\beta_j + \gamma_j) = \exp\left(\sum_{j=1}^{d}\ln(\beta_j + \gamma_j)\right) \le \exp\left(2\sum_{j=1}^{d}\gamma_j\right),$$

where we used that $\beta_j = 1 + \gamma_j$ and $\ln(1+x) \le x$ for any $x > -1$. Recalling that the weights were assumed to be summable, by denoting $\Gamma := \sum_{j=1}^{\infty}\gamma_j$, it follows that

$$\prod_{j=1}^{d}(\beta_j + \gamma_j) \le e^{2\Gamma},$$

which shows that the implied constant of (5.15) is independent of the dimension, but dependent on the weights. From (5.14), (5.15) and using that $1/\varphi(n) = O(n^{-1}\ln\ln(n+1))$ with an absolute implied constant (see [46]), we now obtain

$$L_{n,d,\boldsymbol{\gamma}} \le \frac{n-1}{n}\prod_{j=1}^{d}\beta_j + O\left(\frac{\ln\ln(n+1)}{n}\right).$$

By combining the last inequality with (5.7), we obtain

$$M_{n,d,\boldsymbol{\gamma}} \le \frac{1}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n) + O\left(\frac{\ln\ln(n+1)}{n}\right),$$

and hence the result is proved. □

Corollary 5.2 *Let $n \ge 2$ be an integer. If the weights $\{\gamma_j\}_{j=1}^{\infty}$ are summable, then there exists a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

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

where the implied constant depends on the weights, but is independent of the dimension.

Proof. Clearly, there must be a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that $e_{n,d}^2(\boldsymbol{z}) \le M_{n,d,\boldsymbol{\gamma}}$ and the result then follows from Theorem 5.1. □

As we have already mentioned in the previous chapters, in an unweighted setting there exist d-dimensional lattice rules having $O(n^{-1}(\ln n)^d)$ star discrepancy with the implied constant depending only on d and such a bound is widely believed to be the best possible. Under the assumptions made within this chapter, from (5.2), (5.4) and Corollary 5.2, together with $S_n \le 2\ln n$ for any $n \ge 2$ (see (2.24)), it will follow that there exists a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that

$$D_{n,\boldsymbol{\gamma}}^{*}(\boldsymbol{z}) = O(n^{-1}(\ln\ n)^d),$$

but with the implied constant independent of d. A bound that does not involve $\ln n$ is possible by making use of Theorem 3.4 (see also [20, Lemma 3]). This theorem leads to the conclusion that if the weights are summable, then there

exists a generating vector $\boldsymbol{z}$ such that the weighted star discrepancy achieves the strong tractability error bound

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = O(n^{-1+\delta}),$$

for any $\delta > 0$, where the implied constant depends on δ and the weights but is independent of n and d.

Let us also remark that corresponding results for a weighted L_p star discrepancy can be deduced, since such a discrepancy is bounded by the discrepancy introduced in (5.1). Further details can be found in Section 3.6 and [29].

5.3 A component-by-component construction

Before presenting the main result regarding the CBC construction, we need the following:

Lemma 5.3 *There exists a positive constant c independent of n such that*

$$\sum_{k=1}^{n-1} \frac{|T_n(k)|}{\varphi(n)} \leq c \ln n,$$

where $T_n(k)$ is given by (5.6).

Proof. Since $J_n(k) = H_n(k)/\varphi(n) \geq 0$, then from (5.12), we obtain:

$$\sum_{k=1}^{n-1} \frac{|T_n(k)|}{\varphi(n)} \leq \sum_{k=1}^{n-1} \left(2J_n(k) + \frac{|V_n(k)|}{\varphi(n)} \right). \tag{5.16}$$

From the proof of [42, Theorem 5.10], we have

$$\sum_{k=1}^{n-1} J_n(k) = \ln n. \tag{5.17}$$

In order to analyse the second term of (5.16), we see from (5.11) that

$$|V_n(k)| \leq \sum_{a|n} \left| \mu\left(\frac{n}{a}\right) \right| (a,k) \left| \varepsilon\left(\frac{n(a,k)}{a}\right) \right|.$$

By using that $|\varepsilon(m)| < 4m^{-2}$ (see Lemma 2.9), we next obtain:

$$|V_n(k)| \leq 4 \sum_{a|n} \left| \mu\left(\frac{n}{a}\right) \right| \left(\frac{a}{n}\right)^2 = 4 \sum_{a|n} \frac{1}{a^2} \leq \frac{2\pi^2}{3}.$$

Recalling that $1/\varphi(n) = O(\ln\ln(n+1)/n)$ with an absolute implied constant, we now deduce that there exists a constant $c_1 > 0$ independent of n such that

$$\sum_{k=1}^{n-1} \frac{|V_n(k)|}{\varphi(n)} \leq (n-1)\frac{2\pi^2 c_1}{3}\frac{\ln\ln(n+1)}{n} \leq \frac{2\pi^2 c_1 \ln n}{3}.$$

From this inequality combined with (5.16) and (5.17), we obtain:

$$\sum_{k=1}^{n-1} \frac{|T_n(k)|}{\varphi(n)} \leq \left(2 + \frac{2\pi^2 c_1}{3}\right)\ln n,$$

which leads to the desired result by taking $c = 2 + 2\pi^2 c_1/3$. □

As in Chapters 2 and 3, in order to construct the generating vector $\boldsymbol{z}$, we use the component-by-component (CBC) technique. The central idea is to prove that the CBC algorithm produces a generating vector whose corresponding weighted star discrepancy has the same order of magnitude as the bound given in Corollary 5.2. Let us first recall the CBC algorithm:

Component-by-component (CBC) algorithm

The generating vector $\boldsymbol{z} = (z_1, z_2, \ldots, z_d)$ can be constructed as follows:

1. Set the value for the first component of the vector, say $z_1 := 1$.

2. For $m = 2, 3, \ldots, d$, find $z_m \in \mathcal{Z}_n$ such that $e^2_{n,m}(z_1, z_2, \ldots, z_m)$ is minimised, where

$$e^2_{n,m}(z_1, z_2, \ldots, z_m) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{m}(\beta_j + \gamma_j C_k(z_j)) - \prod_{j=1}^{m}\beta_j.$$

The following theorem and corollary will justify the use of the CBC algorithm.

Theorem 5.4 *Let $n \geq 2$ be an integer and suppose that the weights $\{\gamma_j\}_{j=1}^{\infty}$ are summable. If there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

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

where $\alpha = 2 + c$ with c as in Lemma 5.3, then there exists a $z_{d+1} \in \mathcal{Z}_n$ such that

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

Such a z_{d+1} can be found by minimising $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over the set $\mathcal{Z}_n$.

Proof. For any $z_{d+1} \in \mathcal{Z}_n$, we see from (5.5) that

$$\begin{aligned} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) &= \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j C_k(z_j)\right)\left(\beta_{d+1} + \gamma_{d+1}C_k(z_{d+1})\right) \\ &\qquad -\beta_{d+1}\prod_{j=1}^{d}\beta_j \\ &= \beta_{d+1}e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j C_k(z_j)\right)C_k(z_{d+1}) \\ &= \beta_{d+1}e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}S_n}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n) \\ &\quad + \frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j C_k(z_j)\right)C_k(z_{d+1}), \end{aligned}$$

where in the last step the $k = 0$ term has been separated out. Next we average $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over all the possible values of z_{d+1} to form

$$\begin{aligned} \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) &= \frac{1}{\varphi(n)}\sum_{z_{d+1}\in\mathcal{Z}_n} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \\ &= \beta_{d+1}e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}S_n}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n) \\ &\quad + \frac{\gamma_{d+1}}{n\varphi(n)}\sum_{z_{d+1}\in\mathcal{Z}_n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\beta_j + \gamma_j C_k(z_j)\right)C_k(z_{d+1}) \\ &= \beta_{d+1}e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}S_n}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n) \\ &\quad + \frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\left(\frac{1}{\varphi(n)}\sum_{z_{d+1}\in\mathcal{Z}_n} C_k(z_{d+1})\right)\prod_{j=1}^{d}(\beta_j + \gamma_j C_k(z_j)). \end{aligned}$$

From (5.6), it is easy to see that

$$\left|\sum_{z_{d+1}\in\mathcal{Z}_n} C_k(z_{d+1})\right| = |T_n(k)|.$$

It is also obvious that $|C_k(z)| \le S_n$ for any $1 \le k \le n-1$. Using these observations in the last term of the previous inequality, we obtain

$$\begin{aligned} \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) &\le \beta_{d+1}e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1}S_n}{n}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n) \\ &\quad + \frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\frac{|T_n(k)|}{\varphi(n)}\prod_{j=1}^{d}(\beta_j + \gamma_j S_n). \end{aligned}$$

From (2.24) we have $S_n \leq 2\ln n$ and since $\alpha \geq 2$, we obtain $S_n \leq \alpha \ln n$. We can now write

$$\begin{aligned}
\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) &\leq \beta_{d+1} e^2_{n,d}(\boldsymbol{z}) + \frac{\gamma_{d+1} S_n}{n} \prod_{j=1}^{d} (\beta_j + \gamma_j S_n) \\
&\quad + \frac{c\gamma_{d+1} \ln n}{n} \prod_{j=1}^{d} (\beta_j + \gamma_j S_n) \\
&\leq \beta_{d+1} e^2_{n,d}(\boldsymbol{z}) + \frac{(2+c)\gamma_{d+1} \ln n}{n} \prod_{j=1}^{d} (\beta_j + \gamma_j S_n) \\
&\leq \beta_{d+1} e^2_{n,d}(\boldsymbol{z}) + \frac{\alpha\gamma_{d+1} \ln n}{n} \prod_{j=1}^{d} (\beta_j + \alpha\gamma_j \ln n)\,.
\end{aligned}$$

By making use of the hypothesis, we finally obtain

$$\begin{aligned}
\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) &\leq \frac{\beta_{d+1}}{n} \prod_{j=1}^{d} (\beta_j + \alpha\gamma_j \ln n) \\
&\quad + \frac{\alpha\gamma_{d+1} \ln n}{n} \prod_{j=1}^{d} (\beta_j + \alpha\gamma_j \ln n) \\
&= \frac{1}{n} \prod_{j=1}^{d+1} (\beta_j + \alpha\gamma_j \ln n)\,.
\end{aligned}$$

It is obvious that the $z_{d+1} \in \mathcal{Z}_n$ chosen to minimise $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ will satisfy

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

This, together with the previous inequality completes the proof. □

Corollary 5.5 *Let $n \geq 2$ be an integer. If the weights $\{\gamma_j\}_{j=1}^{\infty}$ are summable, then for any $m = 1, 2, \ldots, d$, there exists a $\boldsymbol{z} \in \mathcal{Z}_n^m$ such that*

$$e^2_{n,m}(z_1, z_2, \ldots, z_m) \leq \frac{1}{n} \prod_{j=1}^{m} (\beta_j + \alpha\gamma_j S_n)\,.$$

We can set $z_1 = 1$ and for every $2 \leq m \leq d$, z_m can be chosen by minimising $e^2_{n,m}(z_1, z_2, \ldots, z_m)$ over the set $\mathcal{Z}_n$.

Proof. For $d = 1$, then we see from (2.9) that we have

$$R_n(z, \mathfrak{u}) = \frac{1}{n} \sum_{k=0}^{n-1} \left(1 + {\sum_{-n/2 < h \leq n/2}}' \frac{e^{2\pi \mathrm{i} h k z/n}}{|h|} \right) - 1 = \frac{1}{n} {\sum_{-n/2 < h \leq n/2}}' \sum_{k=0}^{n-1} \frac{(e^{2\pi \mathrm{i} h z/n})^k}{|h|}.$$

Since $h \leq n/2$ and $(z, n) = 1$, it follows that hz cannot be a multiple of n. It is then easy to check using (2.22) that $R_n(z, \mathfrak{u}) = 0$. Hence for $m = 1$ we have $e^2_{n,1}(z_1) = 0$. The result then follows immediately from Theorem 5.4. $\square$

The analysis of the complexity of the CBC construction is similar to the analysis done in Chapter 3. However for completeness, we review the main ideas here. Let's observe first that each $e^2_{n,m}(z_1, z_2, \ldots, z_m)$ can be evaluated in $O(n^2 m)$ operations. This cost can be reduced to $O(nm)$ by using asymptotic techniques as presented in Appendix A and [31]. Consequently, the total complexity of the algorithm will be $O(n^2 d^2)$. This can be reduced to $O(n^2 d)$ if we store the products (see Chapter 3) during the construction at an extra expense of $O(n)$. However, this order of magnitude can be further reduced to $O(nd \log n)$ by using the fast construction proposed in [43]. In the mentioned paper [43] the authors proved that the fast construction algorithm works also in the case when n is not prime (as is the case in this chapter). The central idea of the fast algorithm is based on a fast matrix-vector multiplication and consists of minimising a function of the form

$$\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(1 + \gamma_j \omega \left(\left\{\frac{k z_j}{n}\right\}\right)\right) - 1,$$

where in our situation we can take

$$\omega(x) = \sum_{-\frac{n}{2} < h \leq \frac{n}{2}}{}' \frac{e^{2\pi \mathrm{i} h x}}{|h|}, x \in [0, 1].$$

Thus, with some modifications, the techniques used in [43] will also work here.

Chapter 6

Shifted lattice rules for approximation of integrals over Euclidean space in weighted reproducing kernel Hilbert spaces

In this chapter we study the problem of approximating weighted integrals over Euclidean space with the weight function being a probability density. The function space considered here is a reproducing kernel Hilbert space with the kernel based on Fourier transforms. After defining the worst-case error, we prove that by mapping $\mathbb{R}^d$ to the unit cube, we can construct shifted lattice rules over the unit cube such that our defined mean worst-case error is of order $O(n^{-1/2})$, where, under appropriate conditions on the weights, the involved constant is independent of the dimension. We also perform numerical experiments on the error resulting from the use of these shifted lattice rules. These numerical experiments seem to suggest that in practice, the order of convergence for the error is better than the theoretical $O(n^{-1/2})$.

6.1 Introduction

Integrals over Euclidean space given by

$$\int_{\mathbb{R}^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{6.1}$$

have been studied in [51, Chapter 9.3], [54] and [59]. In those works, it was assumed that f is a smooth function that decays rapidly at infinity. The quadrature rule proposed to approximate such integrals was of the form

$$Q(f) = \det L \sum_{\boldsymbol{x}\in L} f(\boldsymbol{x}),$$

where $L \subset \mathbb{R}^d$ was an infinite lattice as defined in Chapter 1 by Definition 1.1, while $\det L$ denoted the "determinant" of the lattice, that is, the volume of the unit cell or equivalently, the reciprocal of the point density of the lattice. Let's assume that the function f has the Fourier transform given by

$$\hat{f}(\boldsymbol{w}) = \int_{\mathbb{R}^d} f(\boldsymbol{x}) e^{-2\pi \mathrm{i}\boldsymbol{w}\cdot\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x}.$$

When $\hat{f} \in L_1$, we also have

$$f(\boldsymbol{x}) = \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{w}) e^{2\pi \mathrm{i}\boldsymbol{w}\cdot\boldsymbol{x}}\,\mathrm{d}\boldsymbol{w}.$$

From [51, Theorem 9.9] or [54, Theorem 1], it turned out that if f and the Fourier coefficients $\hat{f}$ satisfy the conditions $|f(\boldsymbol{x})| \leq c(1 + ||\boldsymbol{x}||_E)^{-d-\delta}$ and $|\hat{f}(\boldsymbol{w})| \leq c_1(1 + ||\boldsymbol{w}||_E)^{-d-\delta}$ for some constants c, c_1 and $\delta > 0$, where $||\cdot||_E$ is the usual Euclidean norm, then the quadrature error can be expressed as

$$Q(f) - \int_{\mathbb{R}^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \sum_{\boldsymbol{w}\in L^\perp}{}' \hat{f}(\boldsymbol{w}),$$

where by $L^\perp$ we denote the dual of the lattice L (see Definition 2.1). Later in [51, Section 9.3] or [54, Section 3], it was shown that the "best" lattice among those with a given determinant to be chosen for a good approximation of integrals given by (6.1), is the one whose dual lattice has the densest sphere packing. In simple terms, the density of the sphere packing represents the fraction of the total volume occupied by a packing of spheres of the same radius

without overlapping. Generator matrices for lattices with densely packed duals can be found in [5] and [58] and further details on the sphere packing density can also be found in these two works.

Although the criterion based on the sphere packing density seems to be very appealing, there are technical difficulties that arise almost immediately. For instance, there is a lack of practical algorithms that could be used to calculate the density of a sphere packing. Such algorithms, if any, are at least NP-difficult or conjectured to be in the class of NP-hard problems as shown in [5]. Secondly, lattices with the densest sphere packing are not known for *every* given dimension. In fact, lattices with the densest possible sphere packing are known for $d = 2, 3, 4, 5, 6, 7, 8$ (details on such lattices can be found in [58]). The website http://www.research.att.com/~njas/lattices/density.html contains tables of available lattices with the densest sphere packing known up to dimension 48 and then for $d = 54, 56, 64, 80$ and 128.

Due to the difficulties described above, instead of considering integrals of the form (6.1), we shall consider in the rest of this chapter integrals over Euclidean space given by (see also (1.4))

$$I_d(f, \rho) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

where $\rho(\boldsymbol{x})$ is a probability density function. Hence $\rho(\boldsymbol{x}) \geq 0$ for any $\boldsymbol{x} \in \mathbb{R}^d$ and $\int_{\mathbb{R}^d} \rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 1$. We also assume that the probability density is of the product form

$$\rho(\boldsymbol{x}) = \prod_{j=1}^{d} \rho_j(x_j),$$

where each ρ_j is a probability density over $\mathbb{R}$. For convenience, we shall also assume that all the ρ_j are equal. However the results can be extended in the case when the densities ρ_j are different for each coordinate direction.

Integrals over unbounded regions may be studied by first employing a mapping to the unit cube (see [21], [22], [23]) and then generating a shifted lattice rule over the unit cube. Such a technique has been used in [38] and [62]. In

the 1-dimensional case, we can use the following transform:

$$u = \Phi(x) = \int_{-\infty}^{x} \rho(t)\,\mathrm{d}t, \quad \forall x \in \mathbb{R}. \tag{6.2}$$

The inverse mapping will be $\Phi^{-1} : (0,1) \to \mathbb{R}, \quad \Phi^{-1}(u) = x$. Let's observe that if Φ is differentiable, then $\Phi'(x) = \rho(x), \quad \forall x \in \mathbb{R}$. In the d-dimensional case, the mapping (6.2) will be applied for each coordinate direction. Hence, if $\boldsymbol{x} = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, then $\Phi(\boldsymbol{x}) = (\Phi(x_1), \Phi(x_2), \ldots, \Phi(x_d))$. In the same manner, the inverse mapping will also be applied component-wise. The integral (1.4) will thus become

$$I_d(f,\rho) = \int_{[0,1]^d} f(\Phi^{-1}(\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u} = \int_{[0,1]^d} g(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u},$$

where $g = f \circ \Phi^{-1}$ (applied component-wise). These integrals can be approximated by quadrature rules of the form

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

where $\boldsymbol{t}_k = \Phi^{-1}(\boldsymbol{w}_k) \in \mathbb{R}^d$, for all $0 \le k \le n-1$.

Next, we give some examples of possible choices for the density $\rho(\boldsymbol{x})$ and establish some further properties of the transform (6.2). These densities were also considered in [38].

Example 1 Consider the Gaussian distribution on $\mathbb{R}$ defined by

$$\rho(x) = \frac{1}{\sqrt{2\pi\lambda}} e^{-\frac{x^2}{2\lambda}}, \quad \lambda > 0.$$

Such a distribution occurs frequently in applications and was used for instance in [62].

Example 2 The two-tailed exponential distribution on $\mathbb{R}$ defined by

$$\rho(x) = \frac{1}{2\lambda} e^{-\frac{|x|}{\lambda}}, \quad \lambda > 0.$$

This distribution will be considered for the numerical experiments given later in this chapter.

Example 3 For any $x \in \mathbb{R}$, consider

$$\rho(x) = \frac{\lambda - 1}{2(1+|x|)^{\lambda}}, \quad \lambda > 1.$$

Let's remark that the densities considered in the previous three examples are even functions, that is $\rho(x) = \rho(-x)$, $\forall x \in \mathbb{R}$. For such densities, the transform defined by (6.2) will satisfy

$$\Phi(-x) = 1 - \Phi(x), \quad \forall x \in \mathbb{R}. \tag{6.3}$$

Consequently, the inverse transform will satisfy

$$\Phi^{-1}(1-u) = -\Phi^{-1}(u), \quad \forall u \in (0,1). \tag{6.4}$$

Both (6.3) and (6.4) are easy to prove and will be useful later in this chapter. Let's also remark that the derivative of Φ^{-1} is given by

$$(\Phi^{-1}(u))' = \frac{1}{\rho(\Phi^{-1}(u))}.$$

It is easy to see that the function Φ is increasing and hence Φ^{-1} is increasing too.

The rest of the chapter is structured as follows: in the next section, we consider reproducing kernel Hilbert spaces and review briefly some concepts of the theory of reproducing kernels. Reproducing kernel Hilbert spaces were considered in numerous other research papers devoted to quasi-Monte Carlo methods for multiple integration. These papers include but are not limited to [8], [9], [25], [35], [36], [37], [38], [52], [57], and [62]. Since earlier in this section we mentioned that the quadrature error can be expressed in terms of the Fourier coefficients, it seems natural to use a reproducing kernel based on the Fourier transform of functions. After defining a worst-case error and introducing the weights, we construct shifted lattice rules in the unit cube using the usual CBC technique. By using the inverse mapping Φ^{-1}, we obtain a quadrature rule containing points from the whole Euclidean space that can be used to approximate weighted integrals over $\mathbb{R}^d$. Then, we establish that if the weights are summable, the order of magnitude of the error is $O(n^{-1/2})$ with the involved constant independent of the dimension, and hence we achieve

strong tractability. Although the theoretical convergence is the same as for Monte Carlo methods, our numerical tests seem to suggest that in practice the convergence is better that the theoretical $O(n^{-1/2})$. However, we need to mention that our results are rather speculative and based on some limited numerical experiments. By using a different measure of goodness, a better theoretical convergence will be achieved in the next chapter.

6.2 The function space

Throughout this chapter we assume that the function f admits a Fourier transform $\hat{f}$ and that Fourier inversion also holds as indicated in the previous section. We shall also assume that f belongs to a reproducing kernel Hilbert space and we start this section by recalling some concepts from the theory of reproducing kernels. Further details can be found on [2].

Definition 6.1 *A reproducing kernel Hilbert space H of functions on $\mathbb{R}^d$ is a Hilbert space in which for any $\boldsymbol{y} \in \mathbb{R}^d$, the point evaluation functional*

$$\mathcal{F}_{\boldsymbol{y}}(f) = f(\boldsymbol{y}), \quad \forall f \in H,$$

is a bounded linear functional on H.

If $\langle \cdot, \cdot \rangle$ and $|| \cdot ||$ denote the inner product and respectively, the norm in the space H, then from Riesz's representation theorem (see for instance [4] or [40]), there exists a unique function K defined on $\mathbb{R}^d \times \mathbb{R}^d$ such that

$$\mathcal{F}_{\boldsymbol{y}}(f) = f(\boldsymbol{y}) = \langle f, K(\cdot, \boldsymbol{y}) \rangle, \quad \forall f \in H, \quad \forall \boldsymbol{y} \in \mathbb{R}^d.$$

The function K is known as the "reproducing kernel" of the Hilbert space H. For any other bounded linear functional $\mathcal{F}$, the representer $\tilde{\mathcal{F}}$ satisfying $\mathcal{F} = \langle f, \tilde{\mathcal{F}} \rangle$ is given by

$$\tilde{\mathcal{F}}(\boldsymbol{y}) = \langle \tilde{\mathcal{F}}, K(\cdot, \boldsymbol{y}) \rangle = \mathcal{F}(K(\cdot, \boldsymbol{y})).$$

Definition 6.2 *A reproducing kernel is said to be "shift-invariant" if it has the property*

$$K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{x} + \boldsymbol{\Delta}, \boldsymbol{y} + \boldsymbol{\Delta}), \quad \forall \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\Delta} \in \mathbb{R}^d.$$

It can be checked that the condition $K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{x}+\boldsymbol{\Delta}, \boldsymbol{y}+\boldsymbol{\Delta})$ is equivalent with $K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{x} - \boldsymbol{y}, \boldsymbol{0})$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ (see for instance [25]). If the reproducing kernel is real-valued, then since $\mathcal{F}_{\boldsymbol{y}}(f) = \langle f, K(\cdot, \boldsymbol{y})\rangle$ and by using the symmetry property of the inner product, we obtain:

$$K(\boldsymbol{x}, \boldsymbol{y}) = \langle K(\cdot, \boldsymbol{x}), K(\cdot, \boldsymbol{y})\rangle = \langle K(\cdot, \boldsymbol{y}), K(\cdot, \boldsymbol{x})\rangle = K(\boldsymbol{y}, \boldsymbol{x}),$$

for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$. Hence a real-valued reproducing kernel is symmetric. For complex reproducing kernels, we have

$$K(\boldsymbol{x}, \boldsymbol{y}) = \overline{K(\boldsymbol{y}, \boldsymbol{x})}, \quad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d.$$

As mentioned earlier, more details on the theory of reproducing kernels can be found in [2].

Let us assume that the reproducing kernel K is shift-invariant, so $K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{x} - \boldsymbol{y}, \boldsymbol{0}) = K(\boldsymbol{t}, \boldsymbol{0})$, where we put $\boldsymbol{t} = \boldsymbol{x} - \boldsymbol{y}$. If $K \in L_1$, then the Fourier transform of such a kernel is given by

$$\hat{K}(\boldsymbol{w}) = \int_{\mathbb{R}^d} K(\boldsymbol{t}, \boldsymbol{0}) e^{-2\pi \mathrm{i} \boldsymbol{w}\cdot\boldsymbol{t}} \, \mathrm{d}\boldsymbol{t}.$$

Consequently, if $\hat{K} \in L_1$, then

$$K(\boldsymbol{x} - \boldsymbol{y}, \boldsymbol{0}) = \int_{\mathbb{R}^d} \hat{K}(\boldsymbol{w}) e^{2\pi \mathrm{i} \boldsymbol{w}\cdot(\boldsymbol{x}-\boldsymbol{y})} \, \mathrm{d}\boldsymbol{w} = \int_{\mathbb{R}^d} \hat{K}(\boldsymbol{w}) e^{2\pi \mathrm{i} \boldsymbol{w}\cdot\boldsymbol{t}} \, \mathrm{d}\boldsymbol{w}.$$

We can now prove the following result:

Proposition 6.1 *Let us assume that $K \in L_1$ is a shift-invariant reproducing kernel with the non-negative Fourier transform $\hat{K} \in L_1$. Let f and g be two square integrable functions in H and let us define the inner product*

$$\langle f, g\rangle := \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{w})\overline{\hat{g}(\boldsymbol{w})}}{\hat{K}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w}. \tag{6.5}$$

Then the space of functions satisfying $||f|| < \infty$ is a reproducing kernel Hilbert space, where

$$||f|| = \left(\int_{\mathbb{R}^d} \frac{|\hat{f}(\boldsymbol{w})|^2}{\hat{K}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w} \right)^{1/2}. \tag{6.6}$$

Proof. From Bochner's theorem (see for instance [3] or [40]), it follows that $K(\boldsymbol{t}, \boldsymbol{0})$ is non-negative if and only if $\hat{K}(\boldsymbol{w})$ is non-negative. Since it was assumed that $\hat{K}$ is non-negative, the kernel will be non-negative and it will follow that it is real. From the symmetry property $K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{y}, \boldsymbol{x})$ for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, it also follows that $K(\boldsymbol{t}, \boldsymbol{0}) = K(-\boldsymbol{t}, \boldsymbol{0})$, for any $\boldsymbol{t} \in \mathbb{R}^d$. It is then easy to verify the reproducing property of K. Indeed, since $\hat{K}$ is real, we have

$$\langle f(\cdot), K(\cdot, \boldsymbol{y}) \rangle = \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{w}) \overline{e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{y}} \hat{K}(\boldsymbol{w})}}{\hat{K}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w} = f(\boldsymbol{y}),$$

for any $\boldsymbol{y} \in \mathbb{R}^d$. □

Let us remark that similar assumptions on the kernel and the same norm as (6.6) have been considered in works such as [3] or [63]. These assumptions on the kernel will be valid for the rest of the chapter.

Example. Next, we give an example of such reproducing kernel. In a 1-dimensional space, let us consider $K(x, y) = ce^{-\alpha|x-y|}$ with $c > 0$. It can be checked that

$$\hat{K}(w) = \frac{2c\alpha}{\alpha^2 + 4\pi^2 w^2}.$$

When $c = \pi$ and $\alpha = 2\pi$, we obtain $K(x, y) = \pi e^{-2\pi|x-y|}$ and this will be the kernel chosen for the numerical experiments considered later in this chapter. It turns out that $\hat{K}(w) = (1 + w^2)^{-1}$ and the inner product defined by (6.5) is now given by

$$\langle f, g \rangle := \int_{-\infty}^{\infty} \hat{f}(w) \overline{\hat{g}(w)} (1 + w^2) \, \mathrm{d}w.$$

If f is differentiable and f' is integrable with its Fourier transform given by $\hat{f}'(w) = \int_{-\infty}^{\infty} e^{-2\pi \mathrm{i} w x} f'(x) \, \mathrm{d}x$, then after an integration by parts and under the assumption that $f(x) \to 0$ when $x \to \pm\infty$, we obtain:

$$\hat{f}'(w) = e^{-2\pi \mathrm{i} w x} f(x)|_{-\infty}^{\infty} + (2\pi \mathrm{i} w) \int_{-\infty}^{\infty} e^{-2\pi \mathrm{i} w x} f(x) \, \mathrm{d}x = 2\pi \mathrm{i} w \hat{f}(w).$$

Using (6.6), we obtain

$$||f||^2 = \int_{-\infty}^{\infty} |\hat{f}(w)|^2(1+w^2)\,\mathrm{d}w.$$

If $||f|| < \infty$, then $\int_{-\infty}^{\infty} w^2|\hat{f}(w)|^2\,\mathrm{d}w < \infty$ and from Parseval's theorem (see for instance [40]) together with the expression of the derivative, we obtain

$$\int_{-\infty}^{\infty} |f'(x)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} |\widehat{f'}(w)|^2\,\mathrm{d}w = 4\pi^2 \int_{-\infty}^{\infty} w^2|\hat{f}(w)|^2\,\mathrm{d}w < \infty.$$

Consequently, the corresponding space will consist of functions with square integrable first derivative. In a d-dimensional space, the corresponding space of functions will consist of functions with square-integrable mixed first derivatives. Spaces with square-integrable mixed first derivatives such as weighted Korobov spaces of periodic functions or weighted Sobolev spaces have been previously considered in numerous research papers including [35], [36], [37], [38] and [52].

6.3 Worst-case error

In order to express the integration error, we need first the following result:

Lemma 6.2 *If the linear functionals*

$$I_d(f,\rho) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

and

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

are bounded, then their representers are given by the following functions:

$$h(\boldsymbol{x}) = \int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}, \tag{6.7}$$

and

$$\zeta(\boldsymbol{x}) = \frac{1}{n}\sum_{k=0}^{n-1} K(\boldsymbol{t}_k,\boldsymbol{x}),$$

where the kernel K is satisfying the same assumptions as in Proposition 6.1.

Proof. Using (6.7) and the shift-invariance of K, the Fourier transform of h can be expressed as follows:

$$\begin{aligned}
\hat{h}(\boldsymbol{w}) &= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} K(\boldsymbol{x}, \boldsymbol{y}) \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \right) e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{x}} \, \mathrm{d}\boldsymbol{x} \\
&= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{x}} K(\boldsymbol{x} - \boldsymbol{y}, \boldsymbol{0}) \, \mathrm{d}\boldsymbol{x} \right) \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \\
&= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot (\boldsymbol{y} + \boldsymbol{t})} K(\boldsymbol{t}, \boldsymbol{0}) \, \mathrm{d}\boldsymbol{t} \right) \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \\
&= \int_{\mathbb{R}^d} e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{y}} \left(\int_{\mathbb{R}^d} e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{t}} K(\boldsymbol{t}, \boldsymbol{0}) \, \mathrm{d}\boldsymbol{t} \right) \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \\
&= \int_{\mathbb{R}^d} e^{-2\pi \mathrm{i} \boldsymbol{w} \cdot \boldsymbol{y}} \hat{K}(\boldsymbol{w}) \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} = \hat{K}(\boldsymbol{w}) \hat{\rho}(\boldsymbol{w}).
\end{aligned}$$

From (6.5), it follows that

$$\langle f, h \rangle = \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{w}) \overline{\hat{h}(\boldsymbol{w})}}{\hat{K}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w} = \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{w}) \overline{\hat{K}(\boldsymbol{w}) \hat{\rho}(\boldsymbol{w})}}{\hat{K}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w} = \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{w}) \overline{\hat{\rho}(\boldsymbol{w})} \, \mathrm{d}\boldsymbol{w},$$

and from Parseval's theorem, we obtain

$$\langle f, h \rangle = \int_{\mathbb{R}^d} f(\boldsymbol{x}) \overline{\rho(\boldsymbol{x})} \, \mathrm{d}\boldsymbol{x} = I_d(f, \rho).$$

Hence $h(\boldsymbol{x})$ is the representer of $I_d(f, \rho)$. To prove the second part, let's consider

$$\langle f, \zeta \rangle = \langle f, \frac{1}{n} \sum_{k=0}^{n-1} K(\boldsymbol{t}_k, \boldsymbol{x}) \rangle = \frac{1}{n} \sum_{k=0}^{n-1} \langle f, K(\boldsymbol{t}_k, \cdot) \rangle = Q_{n,d}(f),$$

where in the last step we used the reproducing property of K. □

Using Lemma 6.2, we obtain

$$I_d(f, \rho) - Q_{n,d}(f) = \langle f, h - \zeta \rangle$$

and by applying the Cauchy-Schwarz inequality, it follows that

$$|I_d(f, \rho) - Q_{n,d}(f)| \leq ||f|| \cdot ||h - \zeta||, \tag{6.8}$$

where the equality is attained when f is a multiple of $h - \zeta$. From (6.8), we see that we can measure the error by further analysing the quantity $||h - \zeta||$. Let us define now the quantity

$$e^2_{n,d}(P_n, K) := ||h - \zeta||^2,$$

where $P_n := \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ is the set of quadrature points from $Q_{n,d}(f)$. Since the equality in (6.8) is achieved when f is a multiple of $h - \zeta$, it turns that the quantity $e^2_{n,d}(P_n, K)$ defined above can be viewed as a worst-case error. In papers such as [25], this quantity is also named the "discrepancy". We now establish the following:

Theorem 6.3

$$\begin{aligned} e^2_{n,d}(P_n, K) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x}, \boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{k=0}^{n-1}\int_{\mathbb{R}^d} K(\boldsymbol{t}_k, \boldsymbol{y})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \\ &+ \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K(\boldsymbol{t}_i, \boldsymbol{t}_k). \end{aligned} \tag{6.9}$$

Proof. We have

$$e^2_{n,d}(P_n, K) = \langle h - \zeta, h - \zeta\rangle = \langle h, h\rangle - 2\langle h, \zeta\rangle + \langle \zeta, \zeta\rangle.$$

By using the fact that h and ζ are representers of linear functionals, we obtain:

$$\langle h, h\rangle = I_d(h, \rho) = \int_{\mathbb{R}^d} h(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x}, \boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y},$$

where in the last step we used (6.7) and Fubini's theorem (see for instance [4]). We also have

$$\langle h, \zeta\rangle = Q_{n,d}(h) = \frac{1}{n}\sum_{k=0}^{n-1}\int_{\mathbb{R}^d} K(\boldsymbol{t}_k, \boldsymbol{y})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

Finally,

$$\langle \zeta, \zeta\rangle = Q_{n,d}(\zeta) = \frac{1}{n}\sum_{i=0}^{n-1}\zeta(\boldsymbol{t}_i) = \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1} K(\boldsymbol{t}_i, \boldsymbol{t}_k).$$

Substituting this in the expression for $e^2_{n,d}(P_n, K)$, we obtain (6.9). □

Next, we define a mean over all possible $e^2_{n,d}(P_n, K)$ by

$$M_{n,d} := \int_{(\mathbb{R}^d)^n} e^2_{n,d}(P_n, K)\rho(\boldsymbol{t}_0)\rho(\boldsymbol{t}_1)\ldots\rho(\boldsymbol{t}_{n-1})\,\mathrm{d}\boldsymbol{t}_0\,\mathrm{d}\boldsymbol{t}_1\ldots\,\mathrm{d}\boldsymbol{t}_{n-1}. \tag{6.10}$$

We can now establish the following result:

Theorem 6.4

$$M_{n,d} = \frac{1}{n}\int_{\mathbb{R}^d} K(\boldsymbol{x}, \boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x}, \boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}. \tag{6.11}$$

Proof. From (6.9), we see that $e^2_{n,d}(P_n, K)$ can be written as:

$$\begin{aligned} e^2_{n,d}(P_n,K) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{k=0}^{n-1}\int_{\mathbb{R}^d} K(\boldsymbol{t}_k,\boldsymbol{y})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \\ &+ \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{\substack{k=0\\k\neq i}}^{n-1} K(\boldsymbol{t}_i,\boldsymbol{t}_k) + \frac{1}{n^2}\sum_{i=0}^{n-1} K(\boldsymbol{t}_i,\boldsymbol{t}_i). \end{aligned}$$

Using (6.10), it will follow that

$$\begin{aligned} M_{n,d} &= -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ &+ \frac{n^2-n}{n^2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} + \frac{1}{n}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \end{aligned}$$

which is equivalent with the desired result. □

Let's observe that $M_{n,d} \geq 0$ since all $e^2_{n,d}(P_n, K) \geq 0$. However, this could have also followed from the following argument (see also [25]):

$$||K(\cdot,\boldsymbol{x})|| = \sqrt{\langle K(\cdot,\boldsymbol{x}), K(\cdot,\boldsymbol{x})\rangle} = \sqrt{K(\boldsymbol{x},\boldsymbol{x})},$$

which leads to

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle K(\cdot,\boldsymbol{x}), K(\cdot,\boldsymbol{y})\rangle \leq ||K(\cdot,\boldsymbol{x})|| \cdot ||K(\cdot,\boldsymbol{y})|| \leq \sqrt{K(\boldsymbol{x},\boldsymbol{x})}\cdot\sqrt{K(\boldsymbol{y},\boldsymbol{y})}.$$

By applying the Cauchy-Schwarz inequality for integrals, it then follows:

$$\begin{aligned} &\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ \leq\ &\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \sqrt{K(\boldsymbol{x},\boldsymbol{x})\rho(\boldsymbol{x})\rho(\boldsymbol{y})}\cdot\sqrt{K(\boldsymbol{y},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ \leq\ &\sqrt{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{x})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}}\cdot\sqrt{\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{y},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}} \\ =\ &\sqrt{\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}\cdot\sqrt{\int_{\mathbb{R}^d} K(\boldsymbol{y},\boldsymbol{y})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}}, \end{aligned}$$

which shows that

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \leq \int_{\mathbb{R}^d} K(\boldsymbol{x},\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

As mentioned earlier, in order to generate the quadrature points we will map the Euclidean space to the d-dimensional unit cube. Let's remark that the

transformation (6.2) applied component-wise leads to a space $\mathcal{H}$ of functions on $[0,1]^d$, which is isometric with the space H on $\mathbb{R}^d$. Consequently, we have a kernel over the unit cube defined by

$$K(\boldsymbol{x},\boldsymbol{y}) = K(\Phi^{-1}(\boldsymbol{u}),\Phi^{-1}(\boldsymbol{v})) := \mathcal{K}(\boldsymbol{u},\boldsymbol{v}),$$

for any $\boldsymbol{u},\boldsymbol{v} \in [0,1]^d$, where $\boldsymbol{x} = \Phi^{-1}(\boldsymbol{u})$ and $\boldsymbol{y} = \Phi^{-1}(\boldsymbol{v})$. Now we can define the shift-invariant kernel associated with $\mathcal{K}$ by

$$\mathcal{K}^*(\boldsymbol{u},\boldsymbol{v}) = \int_{[0,1]^d} \mathcal{K}(\{\boldsymbol{u}+\boldsymbol{\Delta}\},\{\boldsymbol{v}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}, \tag{6.12}$$

where the braces indicate that we take only the fractional part of the vector's components. Since $\mathcal{K}$ is shift-invariant, the condition $\mathcal{K}^*(\boldsymbol{u},\boldsymbol{v}) = \mathcal{K}^*(\{\boldsymbol{u}+\boldsymbol{\Delta}\},\{\boldsymbol{v}+\boldsymbol{\Delta}\})$ for any $\boldsymbol{u},\boldsymbol{v},\boldsymbol{\Delta} \in [0,1]^d$ is equivalent with $\mathcal{K}^*(\boldsymbol{u},\boldsymbol{v}) = \mathcal{K}^*(\{\boldsymbol{u}-\boldsymbol{v}\},\boldsymbol{0})$. Hence $\mathcal{K}^*(\boldsymbol{u},\boldsymbol{v})$ depends only on $\{\boldsymbol{u}-\boldsymbol{v}\}$.

Let's define

$$\psi(\boldsymbol{w}) := \mathcal{K}^*(\boldsymbol{w},\boldsymbol{0}) = \mathcal{K}^*(\{\boldsymbol{u}-\boldsymbol{v}\},\boldsymbol{0}),$$

where we put $\boldsymbol{w} = \{\boldsymbol{u}-\boldsymbol{v}\}$ and analyse next the function ψ in the 1-dimensional case. Hence, we now consider the univariate function

$$\psi(w) = \int_0^1 \mathcal{K}(\{w+\Delta\},\Delta)\,\mathrm{d}\Delta. \tag{6.13}$$

Further properties of ψ will be useful at the expression of the worst-case error and mean worst-case error and will also allow us to establish a convexity property of ψ. Such a property will be useful at the construction of the quadrature points. An expression for ψ is given by the following result:

Lemma 6.5 *The function ψ defined above can be written as*

$$\psi(w) = 2\psi_1(w) + 2\psi_1(1-w), \quad \forall w \in (0,1),$$

where

$$\psi_1(w) = \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w+\Phi(t)),t)\rho(t)\,\mathrm{d}t. \tag{6.14}$$

The proof of this lemma is given in Appendix B. Let us remark that a similar result was also established in [62], however it was valid only for the particular

kernel used therein and under the assumption that the probability distribution was Gaussian. Our result here will hence allow slightly more generality, since it will work for more general distributions. This last result also shows that further properties of $\mathcal{K}^*$ and implicitly of K, can be determined by analysing properties of $\psi_1(w)$. For instance, if ψ_1 is twice differentiable, then the first and the second derivatives of ψ could be expressed as follows:

$$\psi'(w) = 2\psi_1'(w) - 2\psi_1'(1-w),$$

and

$$\psi''(w) = 2\psi_1''(w) + 2\psi_1''(1-w). \tag{6.15}$$

For the rest of the chapter, we assume that $\psi_1''(w) \geq 0$, $\forall w \in [0,1]$. A similar result was established in [38] and [62]. From (6.15), we obtain $\psi''(w) \geq 0$ and hence ψ is a convex function. In Appendix B we actually give a proof that ψ is convex for a specific kernel (see Lemma B.1). From [62, Lemma 2], it follows that

$$\frac{1}{n-1}\sum_{i=1}^{n-1}\psi\left(\frac{i}{n}\right) < \int_0^1 \psi(w)\,\mathrm{d}w, \tag{6.16}$$

for any positive integer $n \geq 2$ and we shall assume that (6.16) holds for each individual coordinate $j = 1, \ldots, d$. Let us also mention that the result stated by (6.16) will be used later at the construction of the quadrature points.

6.4 Worst-case error in weighted reproducing kernel Hilbert spaces

As usual, we denote $\mathcal{D} = \{1, 2, \ldots, d\}$ and assume that $\boldsymbol{\gamma}_{\mathfrak{u}}$ is the weight associated with each non-empty subset $\mathfrak{u} \subseteq \mathcal{D}$. We also denote by $K_j(x_j, y_j)$ the 1-dimensional kernel associated with each coordinate j and assume that each such kernel is shift-invariant and non-negative. We now introduce the weighted kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} K_j(x_j, y_j). \tag{6.17}$$

Further assumption on the weights will be made later. Next, we expand the expression of the quadrature error given by (6.9). For each $j = 1, \ldots, d$, let us define

$$C_j := \int_0^1 \mathcal{K}_j(u_j, u_j)\, \mathrm{d}u_j = \int_{-\infty}^{\infty} K_j(x_j, x_j)\rho(x_j)\, \mathrm{d}x_j, \tag{6.18}$$

where we recall that $\mathcal{K}(u, v) = K(\Phi^{-1}(u), \Phi^{-1}(v))$, for any $u, v \in (0, 1)$. We also define

$$D_j := \int_0^1 \int_0^1 \mathcal{K}_j(u_j, v_j)\, \mathrm{d}u_j\, \mathrm{d}v_j = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K_j(x_j, y_j)\rho(x_j)\rho(y_j)\, \mathrm{d}x_j\, \mathrm{d}y_j. \tag{6.19}$$

From the final part of the previous section, it follows that

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K(x, y)\rho(x)\rho(y)\, \mathrm{d}x\, \mathrm{d}y \leq \int_{-\infty}^{\infty} K(x, x)\rho(x)\, \mathrm{d}x,$$

which in turn leads to $C_j \geq D_j$ for each j. At this stage, we shall mention that we may have different 1-dimensional kernels corresponding to each j, but for simplicity and for computational purposes, we assume that all individual 1-dimensional kernels are equal. The same assumption has also been made in [38] and [62] and, as in those papers, the results here could be generalised in the situation when the kernels K_j are different for each j.

Let's assume that the quadrature points are of the form $\boldsymbol{w}_k = \{\frac{k}{n}\boldsymbol{z} + \boldsymbol{\Delta}\}$, for any $k = 0, \ldots, n-1$, where as usual, $z \in \mathcal{Z}_n^d$ denotes the generating vector having all the components assumed to be relatively prime with n, while $\boldsymbol{\Delta} \in [0, 1]^d$ is a randomly chosen shift. Recall from Section 6.3 that $P_n = \{\boldsymbol{t}_0, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{n-1}\}$ is the set of quadrature points in $\mathbb{R}^d$ obtained by using the inverse transformation Φ^{-1} component-wise, where Φ is as given by (6.2). We thus obtain $\boldsymbol{t}_k = \Phi^{-1}(\boldsymbol{w}_k)$, for any $0 \leq k \leq n-1$. Obviously, the quantity $e_{n,d}^2(P_n, K)$ expressed by (6.9) depends on the generating vector $\boldsymbol{z}$ and the shift $\boldsymbol{\Delta}$, so it makes sense to write $e_{n,d}^2(\boldsymbol{z}, \boldsymbol{\Delta}) := e_{n,d}^2(P_n, K)$. With these notations, we see that under the assumption (6.17), the formulae (6.9) and (6.11) proved

in Theorems 6.3 and 6.4 can be written as follows:

$$e^2_{n,d}(\boldsymbol{z},\boldsymbol{\Delta}) = \sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\prod_{j\in\mathfrak{u}}D_j - \frac{2}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}\int_0^1 \mathcal{K}_j(\{kz_j/n+\Delta_j\},u)\,\mathrm{d}u + \frac{1}{n^2}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\sum_{i=0}^{n-1}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}\mathcal{K}_j(\{iz_j/n+\Delta_j\},\{kz_j/n+\Delta_j\}), \quad (6.20)$$

while the mean can be written as

$$M_{n,d} = \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\left(\prod_{j\in\mathfrak{u}}C_j - \prod_{j\in\mathfrak{u}}D_j\right). \quad (6.21)$$

Now we can define a mean worst-case error over all possible $\boldsymbol{\Delta}\in[0,1]^d$ by

$$[e^*_{n,d}(\boldsymbol{z})]^2 := \int_{[0,1]^d} e^2_{n,d}(\boldsymbol{z},\boldsymbol{\Delta})\,\mathrm{d}\boldsymbol{\Delta}.$$

From (6.12) and (6.20) with the notations (6.18) and (6.19), it is easy to see that

$$[e^*_{n,d}(\boldsymbol{z})]^2 = -\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\prod_{j\in\mathfrak{u}}D_j + \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}\mathcal{K}^*_j\left(\left\{\frac{k}{n}z_j\right\},0\right). \quad (6.22)$$

Alternatively, by separating out the $k=0$ term, equation (6.22) can be written as:

$$[e^*_{n,d}(\boldsymbol{z})]^2 = -\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\prod_{j\in\mathfrak{u}}D_j + \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\prod_{j\in\mathfrak{u}}C_j + \frac{1}{n}\sum_{\mathfrak{u}\subseteq\mathcal{D}}\boldsymbol{\gamma}_{\mathfrak{u}}\sum_{k=1}^{n-1}\prod_{j\in\mathfrak{u}}\mathcal{K}^*_j\left(\left\{\frac{k}{n}z_j\right\},0\right). \quad (6.23)$$

For the rest of the chapter we assume that the weights are product (recall that $\boldsymbol{\gamma}_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}}\gamma_j$) and for convenience, we shall also assume that n is prime. As mentioned earlier in this section, the kernels associated with each coordinate are equal. Consequently, all the quantities $\mathcal{K}^*_j(w,0)$ will be equal with $\psi(w)$, where ψ is as given by (6.13). Moreover, $C = C_j$ and $D = D_j$ for all $j = 1,\ldots,d$, where C_j and D_j were defined by (6.18) and (6.19). It is also easy to see from (6.13) that

$$\int_0^1 \psi(w)\,\mathrm{d}w = D.$$

Then the mean worst-case error and the mean given respectively by (6.23) and (6.21) can be rewritten as follows:

$$[e^*_{n,d}(\boldsymbol{z})]^2 = \frac{1}{n}\prod_{j=1}^{d}(1+C\gamma_j) + \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\})) - \prod_{j=1}^{d}(1+D\gamma_j), \quad (6.24)$$

while the mean becomes

$$M_{n,d} = \frac{1}{n}\left(\prod_{j=1}^{d}(1+C\gamma_j) - \prod_{j=1}^{d}(1+D\gamma_j)\right). \tag{6.25}$$

6.5 The construction of the quadrature points

In this section we first prove that there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that $[e^*_{n,d}(\boldsymbol{z})]^2 \le M_{n,d}$ and then construct such a vector using the usual component-by-component (CBC) technique. The existence result is given by the following:

Theorem 6.6 *If n is prime, then there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$[e^*_{n,d}(\boldsymbol{z})]^2 \le \frac{1}{n}\left(\prod_{j=1}^{d}(1+C\gamma_j) - \prod_{j=1}^{d}(1+D\gamma_j)\right).$$

Proof. Since n is prime, there are $(n-1)^d$ possible choices for $\boldsymbol{z}$. If we average $[e^*_{n,d}(\boldsymbol{z})]^2$ over all possible vectors $\boldsymbol{z} \in \mathcal{Z}_n^d$, then by using (6.24) we obtain

$$\begin{aligned}
\frac{1}{(n-1)^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d}[e^*_{n,d}(\boldsymbol{z})]^2 &= \frac{1}{n}\prod_{j=1}^{d}(1+C\gamma_j) - \prod_{j=1}^{d}(1+D\gamma_j) \\
&\quad + \frac{1}{n(n-1)^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\})) \\
&= \frac{1}{n}\prod_{j=1}^{d}(1+C\gamma_j) - \prod_{j=1}^{d}(1+D\gamma_j) \\
&\quad + \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}\left(\frac{1}{n-1}\sum_{z_j=1}^{n-1}(1+\gamma_j\psi(\{kz_j/n\}))\right).
\end{aligned}$$

However the quantities $\{kz_j/n\}$ for $1 \le z_j \le n-1$ are the same as i/n for $i = 1, \ldots, n-1$, but in a different order. Recalling that $\int_0^1 \psi(w)\,\mathrm{d}w = D$, it will follow from (6.16) that

$$\frac{1}{n-1}\sum_{z_j=1}^{n-1}\psi(\{kz_j/n\}) < \int_0^1 \psi(w)\,\mathrm{d}w = D. \tag{6.26}$$

Using (6.26) in the expression for the average, we obtain

$$\frac{1}{(n-1)^d}\sum_{\boldsymbol{z}\in\mathcal{Z}_n^d}[e^*_{n,d}(\boldsymbol{z})]^2 \le \frac{1}{n}\prod_{j=1}^{d}(1+C\gamma_j) - \prod_{j=1}^{d}(1+D\gamma_j) + \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+D\gamma_j) = M_{n,d},$$

where $M_{n,d}$ is as given by (6.25). This proves the existence of a vector $\boldsymbol{z}$ such that $[e^*_{n,d}(\boldsymbol{z})]^2 \leq M_{n,d}$. □

In order to construct $\boldsymbol{z}$, we can use the usual CBC algorithm:

Component-by-component algorithm

1. Set the value for the first component of the vector, say $z_1 = 1$.

2. For $m = 2, 3, \ldots, d$, find $z_m \in \mathcal{Z}_n$ such that $[e^*_{n,m}(z_1, \ldots, z_m)]^2$ is minimised, where

$$[e^*_{n,m}(z_1, \ldots, z_m)]^2 = \frac{1}{n}\prod_{j=1}^{m}(1+C\gamma_j)+\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{m}(1+\gamma_j\psi(\{kz_j/n\}))-\prod_{j=1}^{m}(1+D\gamma_j).$$

The algorithm is based on the following result:

Theorem 6.7 *Let n be prime. Suppose there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$[e^*_{n,d}(\boldsymbol{z})]^2 \leq \frac{1}{n}\left(\prod_{j=1}^{d}(1 + C\gamma_j) - \prod_{j=1}^{d}(1 + D\gamma_j)\right).$$

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

$$[e^*_{n,d+1}(\boldsymbol{z}, z_{d+1})]^2 \leq \frac{1}{n}\left(\prod_{j=1}^{d+1}(1 + C\gamma_j) - \prod_{j=1}^{d+1}(1 + D\gamma_j)\right).$$

Such a z_{d+1} can be found by minimising $[e^*_{n,d+1}(\boldsymbol{z}, z_{d+1})]^2$ over the set $\mathcal{Z}_n$.

Proof. From (6.24), we see that $[e^*_{n,d+1}(\boldsymbol{z}, z_{d+1})]^2$ can be written as:

$$\begin{aligned}
[e^*_{n,d+1}(\boldsymbol{z}, z_{d+1})]^2 &= \frac{1}{n}\prod_{j=1}^{d+1}(1 + C\gamma_j) - \prod_{j=1}^{d+1}(1 + D\gamma_j) + \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d+1}(1 + \gamma_j\psi(\{kz_j/n\})) \\
&= [e^*_{n,d}(\boldsymbol{z})]^2 + \frac{C\gamma_{d+1}}{n}\prod_{j=1}^{d}(1 + C\gamma_j) - D\gamma_{d+1}\prod_{j=1}^{d}(1 + D\gamma_j) \\
&\quad + \frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\psi(\{kz_{d+1}/n\})\prod_{j=1}^{d}(1 + \gamma_j\psi(\{kz_j/n\})).
\end{aligned}$$

Next we average $[e^*_{n,d+1}(\boldsymbol{z}, z_{d+1})]^2$ over all possible values of $z_{d+1} \in \mathcal{Z}_n$ and focus on the last term since it is the only one depending on z_{d+1}. Hence, let's

consider

$$\frac{1}{n-1}\sum_{z_{d+1}=1}^{n-1}\left(\frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\psi(\{kz_{d+1}/n\})\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\}))\right)$$
$$=\frac{\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\left[\left(\frac{1}{n-1}\sum_{z_{d+1}=1}^{n-1}\psi(\{kz_{d+1}/n\})\right)\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\}))\right]$$
$$\leq\frac{D\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\})),$$

where in the last step we used (6.26). From (6.24) and by using the inductive hypothesis, we obtain

$$\begin{aligned}\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\})) &= [e^*_{n,d}(\boldsymbol{z})]^2-\frac{1}{n}\prod_{j=1}^{d}(1+C\gamma_j)+\prod_{j=1}^{d}(1+D\gamma_j)\\ &\leq \prod_{j=1}^{d}(1+D\gamma_j)-\frac{1}{n}\prod_{j=1}^{d}(1+D\gamma_j).\end{aligned}$$

Replacing in the above, we next have

$$\frac{D\gamma_{d+1}}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\}))\leq D\gamma_{d+1}\left(\prod_{j=1}^{d}(1+D\gamma_j)-\frac{1}{n}\prod_{j=1}^{d}(1+D\gamma_j)\right).$$

This result, together with the inductive hypothesis leads to

$$\begin{aligned}\frac{1}{n-1}\sum_{z_{d+1}=1}^{n-1}[e^*_{n,d+1}(\boldsymbol{z},z_{d+1})]^2 &\leq [e^*_{n,d}(\boldsymbol{z})]^2+\frac{C\gamma_{d+1}}{n}\prod_{j=1}^{d}(1+C\gamma_j)\\ &\quad -D\gamma_{d+1}\prod_{j=1}^{d}(1+D\gamma_j)\\ &\quad +D\gamma_{d+1}\left(\prod_{j=1}^{d}(1+D\gamma_j)-\frac{1}{n}\prod_{j=1}^{d}(1+D\gamma_j)\right)\\ &\leq \frac{1}{n}\left(\prod_{j=1}^{d}(1+C\gamma_j)-\prod_{j=1}^{d}(1+D\gamma_j)\right)\\ &\quad +\frac{C\gamma_{d+1}}{n}\prod_{j=1}^{d}(1+C\gamma_j)-\frac{D\gamma_{d+1}}{n}\prod_{j=1}^{d}(1+D\gamma_j)\\ &= \frac{1}{n}\left(\prod_{j=1}^{d+1}(1+C\gamma_j)-\prod_{j=1}^{d+1}(1+D\gamma_j)\right).\end{aligned}$$

Clearly, there must be a $z_{d+1}\in\mathcal{Z}_n$ such that $[e^*_{n,d+1}(\boldsymbol{z},z_{d+1})]^2$ is smaller than the average and obviously, such a z_{d+1} can be found by minimising $[e^*_{n,d+1}(\boldsymbol{z},z_{d+1})]^2$ over $\mathcal{Z}_n$. This completes the proof. □

As in Chapters 2, 3 and 5, the main result on the CBC construction is followed by:

Corollary 6.8 *If n is prime, then for any $1 \le m \le d$ we can construct a vector $\boldsymbol{z} \in \mathcal{Z}_n^m$ component-by-component such that*

$$[e^*_{n,m}(z_1, \ldots, z_m)]^2 \le \frac{1}{n}\left(\prod_{j=1}^{m}(1 + C\gamma_j) - \prod_{j=1}^{m}(1 + D\gamma_j)\right).$$

We can set $z_1 = 1$ and for $2 \le m \le d$, every z_m can be found by minimising $[e^*_{n,m}(z_1, \ldots, z_m)]^2$ over the set $\mathcal{Z}_n$.

Proof. If $m = 1$, it is easy to see that by setting $z_1 = 1$, we obtain

$$[e^*_{n,1}(1)]^2 = \frac{C\gamma_1}{n} + \frac{\gamma_1}{n}\sum_{k=1}^{n-1}\psi(k/n) - D\gamma_1.$$

Using (6.26), it will follow that

$$[e^*_{n,1}(1)]^2 \le \frac{\gamma_1(C - D)}{n}.$$

For $m \ge 2$, the result follows then from Theorem 6.7. □

6.5.1 Strong tractability

Theorem 6.9 *If the weights γ_j satisfy the summability condition*

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

then we can construct the generating vector by using the CBC technique such that the error satisfies the strong tractability bound $e^*_{n,d}(\boldsymbol{z}) = O(n^{-1/2})$, where the involved constant depends on the weights, but independent of the dimension.

Proof. From Theorem 6.7, we see that the generating vector constructed using the CBC technique satisfies

$$[e^*_{n,d}(\boldsymbol{z})]^2 \le \frac{1}{n}\prod_{j=1}^{d}(1 + C\gamma_j) \le \frac{1}{n}\exp\left(\sum_{j=1}^{\infty}\ln(1 + C\gamma_j)\right) \le \frac{1}{n}\exp\left(C\sum_{j=1}^{\infty}\gamma_j\right).$$

Since the weights are summable, it will follow that $e^*_{n,d}(\boldsymbol{z}) = O(n^{-1/2})$, with an absolute implied constant. This ensures strong tractability. □

Let us remark that the order of the magnitude of the error in this chapter is the same as for typical Monte Carlo methods and was also observed in [38] and [62]. In the next chapter however, by using a different criterion of goodness, that is, the weighted discrepancy defined by (2.2), we will construct shifted lattice rules for integrands over Euclidean space that achieve the optimal convergence order of $O(n^{-1+\delta})$ for any $\delta > 0$ and with the involved constant independent of the dimension. Under the condition of summability of the weights (as in Theorem 6.9), this optimal rate of convergence was also obtained in [23]. Here, the convergence order of $O(n^{-1/2})$ follows from the expression of the mean (6.25) and the numerical experiments from the next section confirm that the mean is of order $O(n^{-1})$, which leads to the convergence obtained in Theorem 6.9. The gap between the convergence obtained in this chapter and the convergence attained in [23] and Chapter 7 comes from the fact that here, the measure of goodness used is different from the measure of goodness used in the mentioned works and therefore, different results in terms of convergence might be expected. Nevertheless, particular choices of weights, kernel and density may lead to a better convergence rate than $O(n^{-1/2})$ as some of the numerical experiments from the next section suggest (see Tables 6.16 and 6.17).

6.6 Numerical experiments

6.6.1 Expressions of the error in a particular case

In this section we first find an expression for the quantity $[e^*_{n,d}(\boldsymbol{z})]^2$ given by (6.24) under the assumption that n is prime, the weights are product and, for each j, ρ_j is a two-tailed exponential density given by

$$\rho_j(x) = \pi e^{-2\pi|x|}, \quad \forall x \in \mathbb{R}.$$

We also assume that the kernels associated with each coordinate are equal and each 1-dimensional kernel is given by

$$K(x,y) = \pi e^{-2\pi|x-y|}, \quad \forall x, y \in \mathbb{R}.$$

For this setting, the mapping defined by (6.2) becomes

$$\Phi(x) = \begin{cases} \frac{1}{2}e^{2\pi x}, & x \leq 0, \\ 1 - \frac{1}{2}e^{-2\pi x}, & x > 0. \end{cases}$$

with the inverse $\Phi^{-1} : (0,1) \to \mathbb{R}$ given by

$$\Phi^{-1}(w) = \begin{cases} \frac{1}{2\pi}\ln(2w), & w \leq 1/2, \\ -\frac{1}{2\pi}\ln(2(1-w)), & w > 1/2. \end{cases}$$

Now, we want to determine the expression of the function ψ given by (6.13) in this particular case. Recall from (6.13) that ψ was defined by

$$\psi(w) = 2\psi_1(w) + 2\psi_1(1-w), \quad \forall w \in (0,1),$$

where (see also (6.14))

$$\psi_1(w) = \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w + \Phi(t)), t)\rho(t)\,\mathrm{d}t.$$

For the kernel and the density considered in this subsection, the expression of ψ_1 becomes

$$\psi_1(w) = \pi^2 \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} e^{4\pi t - 2\pi\Phi^{-1}(w+\Phi(t))}\,\mathrm{d}t,$$

where we used that $t \leq \Phi^{-1}((1-w)/2) \leq \Phi^{-1}(1/2) \leq 0$ (recall that Φ^{-1} is increasing). In the situation when $w \leq 1/2$, by using the expressions of Φ and Φ^{-1}, we obtain:

$$\psi_1(w) = \pi^2 \int_{-\infty}^{\frac{\ln(1-2w)}{2\pi}} \frac{e^{4\pi t}}{2w + e^{2\pi t}}\,\mathrm{d}t + \pi^2 \int_{\frac{\ln(1-2w)}{2\pi}}^{\frac{\ln(1-w)}{2\pi}} e^{4\pi t}\left(2(1-w) - e^{2\pi t}\right)\,\mathrm{d}t.$$

In order to calculate the first integral, we may use the change of variable $e^{2\pi t} = y$ to obtain after some elementary calculations that

$$\pi^2 \int_{-\infty}^{\frac{\ln(1-2w)}{2\pi}} \frac{e^{4\pi t}}{2w + e^{2\pi t}}\,\mathrm{d}t = \frac{\pi}{2}\int_0^{1-2w} \frac{y}{2w+y}\,\mathrm{d}y = \frac{\pi}{2} - \pi w + \pi w \ln(2w).$$

We also obtain

$$\pi^2 \int_{\frac{\ln(1-2w)}{2\pi}}^{\frac{\ln(1-w)}{2\pi}} e^{4\pi t} \left(2(1-w) - e^{2\pi t}\right) \,\mathrm{d}t = \frac{\pi w^3}{3} - \pi w^2 + \frac{\pi w}{2}.$$

When $w > 1/2$, we have

$$\psi_1(w) = \pi^2 \int_{-\infty}^{\frac{\ln(1-w)}{2\pi}} e^{4\pi t} \left(2(1-w) - e^{2\pi t}\right) \,\mathrm{d}t = \frac{\pi(1-w)^3}{3}.$$

All these calculations will finally yield

$$\psi(w) = \begin{cases} 2\pi w \ln(2w) + \frac{4\pi w^3}{3} - 2\pi w^2 - \pi w + \pi, & w \le 1/2, \\ 2\pi(1-w)\ln(2(1-w)) + \frac{4\pi(1-w)^3}{3} - 2\pi(1-w)^2 + \pi w, & w > 1/2. \end{cases} \tag{6.27}$$

It is easy to see that if we take $C = C_j$ for any $j = 1, \ldots, d$, where C_j is defined by (6.18), we obtain in this case $C = \pi$. Then by taking $D = D_j$ for any $j = 1, \ldots, d$, where D_j is defined by (6.19), it is relatively easy to check that

$$D = \int_0^1 \psi(w) \,\mathrm{d}w = \frac{3\pi}{8}.$$

Using these values in (6.24), we obtain

$$[e^*_{n,d}(\boldsymbol{z})]^2 = \frac{1}{n}\prod_{j=1}^{d}(1+\pi\gamma_j) + \frac{1}{n}\sum_{k=1}^{n-1}\prod_{j=1}^{d}(1+\gamma_j\psi(\{kz_j/n\})) - \prod_{j=1}^{d}\left(1+\frac{3\pi\gamma_j}{8}\right), \tag{6.28}$$

where the expression of ψ is defined by (6.27), while the corresponding mean (following from (6.25)) is given by

$$M_{n,d} = \frac{1}{n}\left(\prod_{j=1}^{d}(1+\pi\gamma_j) - \prod_{j=1}^{d}(1+3\pi\gamma_j/8)\right). \tag{6.29}$$

The quadrature points in $\mathbb{R}^d$ are given in this case by $\Phi^{-1}(\{\frac{k}{n}\boldsymbol{z} + \boldsymbol{\Delta}\}), k = 0, \ldots, n-1$, where the generating vector $\boldsymbol{z}$ is produced using the CBC technique, $\boldsymbol{\Delta}$ is a randomly chosen shift, and the function Φ^{-1} has the particular expression defined earlier in this subsection.

6.6.2 Tables of numerical results

In this subsection, we calculate the values of (6.28) for several different values of n and d and different choices of weights. We also give values for the mean

(6.29). First, we consider the case when $\gamma_j = 1$ for all $j = 1, \ldots, d$. This corresponds actually to an unweighted case and leads to intractability of the integration problem. The number of points n is prime, while the dimension d takes successively the values $5, 10, 20, 40, 80$. The generating vector $\boldsymbol{z}$ from (6.28) is produced by the CBC technique as presented in Section 6.5.

Table 6.1: $d = 5$ and $\gamma_j = 1$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	6.99463	11.5793
211	2.94906	5.5427
409	1.31503	2.85944
809	0.571254	1.44562
1009	0.427166	1.15908
2003	0.176599	0.583879
4001	0.0721177	0.292305
8009	0.0298932	0.146025
16001	0.0120045	0.0730898
32003	0.00480581	0.0365438

Table 6.2: $d = 10$ and $\gamma_j = 1$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	14094.4	14677.4
211	6634.53	7025.67
409	3353.5	3624.49
809	1656.51	1832.41
1009	1316.75	1468.19
2003	644.531	740.098
4001	310.024	370.512
8009	148.87	185.094
16001	71.3972	92.6453
32003	33.7589	46.3212

Table 6.3: $d = 20$ and $\gamma_j = 1$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	2.18256e+10	2.18286e+10
211	1.04464e+10	1.04487e+10
409	5.38853e+09	5.394043e+09
809	2.72378e+09	2.7252e+09
1009	2.18373e+09	2.18502e+09
2003	1.09975e+09	1.10069e+09
4001	5.50353e+08	5.51033e+08
8009	2.74799e+08	2.75276e+08
16001	1.37459e+08	1.37784e+08
32003	6.86658e+07	6.88899e+07

Table 6.4: $d = 40$ and $\gamma_j = 1$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	4.81253e+22	4.81253e+22
211	2.30363e+22	2.30363e+22
409	1.18843e+22	1.18843e+22
809	6.00823e+21	6.00823e+21
1009	4.8173e+21	4.8173e+21
2003	2.42669e+21	2.42669e+21
4001	1.21486e+21	1.21486e+21
8009	6.069e+20	6.069e+20
16001	3.0377e+20	3.0377e+20
32003	1.51881e+20	1.51881e+20

Table 6.5: $d = 80$ and $\gamma_j = 1$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	2.33921e+47	2.33921e+47
211	1.11972e+47	1.11972e+47
409	5.77653e+46	5.77653e+46
809	2.9204e+46	2.9204e+46
1009	2.34153e+46	2.34153e+46
2003	1.17953e+46	1.17953e+46
4001	5.90503e+45	5.90503e+45
8009	2.94993e+45	2.94993e+45
16001	1.47653e+45	1.47653e+45
32003	7.38244e+44	7.38244e+44

The previous tables clearly illustrate the "curse of dimensionality". While for lower dimensions an increase in the number of points will still produce a reasonable accuracy, it is clear that for higher dimension the number of points needs to be astronomical in order to get some precision. The situation changes dramatically when the weights are summable. Next, we consider the situation when $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

Table 6.6: $d = 5$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0205263	0.0975159
211	0.00696686	0.0466782
409	0.0026932	0.024081
809	0.00101287	0.0121744
1009	0.00072806	0.00976126
2003	0.000265663	0.00491718
4001	9.70102e-05	0.00246166
8009	3.46441e-05	0.00122976
16001	1.18865e-05	0.000615531
32003	4.30286e-06	0.000307756

Table 6.7: $d = 10$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0368221	0.133733
211	0.0132823	0.0640142
409	0.00543038	0.0330244
809	0.00212163	0.0166959
1009	0.00157304	0.0133865
2003	0.000618628	0.00674338
4001	0.000231153	0.0033759
8009	8.78336e-05	0.00168648
16001	3.26577e-05	0.000844134
32003	1.24642e-05	0.000422054

Table 6.8: $d = 20$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0496995	0.158435
211	0.0184875	0.0758386
409	0.00775597	0.0391246
809	0.00309886	0.0197799
1009	0.00231906	0.0158592
2003	0.000942603	0.00798899
4001	0.000360766	0.00399949
8009	0.000141603	0.001998
16001	5.46173e-05	0.00100006
32003	2.1367e-05	0.000500014

Table 6.9: $d = 40$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0578193	0.172915
211	0.0219341	0.08277
409	0.00929782	0.0427004
809	0.00309886	0.0215877
1009	0.00283022	0.0173087
2003	0.00116163	0.00871915
4001	0.000452031	0.00436502
8009	0.000180168	0.0021806
16001	7.0709e-05	0.00109146
32003	2.81424e-05	0.000545713

Table 6.10: $d = 80$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0623542	0.18076
211	0.0238834	0.0865427
409	0.010193	0.0446375
809	0.0041657	0.022567
1009	0.00313443	0.0180939
2003	0.00129345	0.00911469
4001	0.00050729	0.00456304
8009	0.000203788	0.00227953
16001	8.06738e-05	0.00114097
32003	3.23533e-05	0.000570469

Finally we consider the case when the weights are given by $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$. It is easy to see that in this case the weights are also summable. The results are presented in the tables below.

Table 6.11: $d = 5$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.011251	0.0571408
211	0.00384624	0.0273518
409	0.00146383	0.0141106
809	0.000549198	0.00713378
1009	0.000392754	0.00571975
2003	0.000143392	0.00288129
4001	5.17316e-05	0.00144245
8009	1.81757e-05	0.000720593
16001	6.28089e-06	0.000360679
32003	2.20521e-06	0.000180334

Table 6.12: $d = 10$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0140835	0.0643563
211	0.0049524	0.0308056
409	0.00193468	0.0158924
809	0.000739244	0.0080346
1009	0.000535508	0.00644201
2003	0.000199983	0.00324513
4001	7.33784e-05	0.00162459
8009	2.65775e-05	0.000811586
16001	9.55784e-06	0.000406224
32003	3.45789e-06	0.000203106

Table 6.13: $d = 20$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0141905	0.0646055
211	0.00499474	0.0309249
409	0.00195307	0.0159539
809	0.000746633	0.0080657
1009	0.000541042	0.00646695
2003	0.00020225	0.00325769
4001	7.42746e-05	0.00163088
8009	2.69324e-05	0.000814727
16001	9.69766e-06	0.000407797
32003	3.5124e-06	0.000203892

Table 6.14: $d = 40$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0141906	0.0646057
211	0.00499749	0.030925
409	0.00195308	0.015954
809	0.00074664	0.00806573
1009	0.000541047	0.00646697
2003	0.000202253	0.0032577
4001	7.42756e-05	0.00163089
8009	2.69327e-05	0.000814731
16001	9.69781e-06	0.000407798
32003	3.51246e-06	0.000203893

Table 6.15: $d = 80$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	$M_{n,d}$
101	0.0141906	0.0646057
211	0.00499479	0.030925
409	0.00195308	0.015954
809	0.00074664	0.00806573
1009	0.000541047	0.00646697
2003	0.000202253	0.0032577
4001	7.42756e-05	0.00163089
8009	2.69327e-05	0.000814731
16001	9.69781e-06	0.000407798
32003	3.51246e-06	0.000203893

If the weights are summable, then Theorem 6.9 yields the theoretical convergence rate of $O(n^{-1/2})$, with the involved constant independent of the dimension. For some of the numerical results performed above, we have calculated the actual convergence rate one may obtain. In the tables below, the order of convergence is $O(n^{\alpha})$, with

$$\alpha = \frac{\ln(e^*_{n_1,d_1}(\boldsymbol{z}_1)/e^*_{n_2,d_2}(\boldsymbol{z}_2))}{\ln(n_1/n_2)},$$

where $e^*_{n_1,d_1}(\boldsymbol{z}_1)$ and $e^*_{n_2,d_2}(\boldsymbol{z}_2)$ are two consecutive values for $e^*_{n,d}(\boldsymbol{z})$. We see from the tables below that the expected convergence rate is better that the theoretical $O(n^{-1/2})$ given in Theorem 6.9.

Table 6.16: $d = 40$ and $\gamma_j = 1/j^2$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	α
1009	0.00283022	-0.649
2003	0.00116163	-0.682
4001	0.000452031	-0.662
8009	0.000180168	-0.675
16001	7.0709e-05	-0.665
32003	2.81424e-05	

Table 6.17: $d = 80$ and $\gamma_j = (0.5)^j$ for all $j = 1, \ldots, d$.

n	$[e^*_{n,d}(\boldsymbol{z})]^2$	α
1009	0.000541047	-0.711
2003	0.000202253	-0.724
4001	7.42756e-05	-0.731
8009	2.69327e-05	-0.738
16001	9.69781e-06	-0.732
32003	3.51246e-06	

Since the inverse transform Φ^{-1} maps the points generated in the unit cube to the whole Euclidean space, we also tested to find the region where the quadrature points obtained by the CBC construction are located. Let us denote

$$r := \max_{k=0,1,\ldots,n-1} ||\Phi^{-1}(\{k\boldsymbol{z}/n + \boldsymbol{\Delta}\})||_E, \tag{6.30}$$

where $||\cdot||_E$ is the usual Euclidean norm mentioned also in Section 6.1.

As it was pointed out for instance in [11], in order to approximate integrals over Euclidean space, one may truncate the domain to a bounded region, but the size of such a region would be depending on the specific integrand. Of course, in practice a truncation of the domain is performed anyway. Since the error given by (6.28) depends on the quadrature points and not on the actual integrand, we calculated the quantity r given by (6.30) for the values of n and d considered in the experiments performed earlier. The conclusion is that all the quadrature points will be located within a ball centred in the origin with radius r, where r is given by (6.30).

We considered the three choices of weights as earlier in this section. Thus, we first took $\gamma_j = 1$, for any $j = 1, \ldots, d$. Then we considered the two situations when the weights were summable (so the weights satisfy the strong tractability condition from Theorem 6.9). Hence we considered $\gamma_j = 1/j^2$, for any $j = 1, \ldots, d$ and $\gamma_j = (0.5)^j$, for any $j = 1, \ldots, d$. As we see from the table below, the points aren't too far away from the origin, not even for bigger values of n and d.

Table 6.18: Values of r

n	d	r $(\gamma_j = 1)$	r $(\gamma_j = 1/j^2)$	r $(\gamma_j = (0.5)^j)$
101	5	1.23158	1.09515	1.21988
	10	1.25101	1.38088	1.45914
	20	1.61088	1.63756	1.52158
	40	2.20642	2.23058	2.17847
	80	2.67597	2.70681	2.84182
211	5	1.26351	1.23217	1.24361
	10	1.69231	1.52691	1.42816
	20	2.11302	2.39131	2.10961
	40	2.33284	2.09402	2.12308
	80	2.57414	2.72863	2.66407
409	5	1.36937	1.41171	1.41171
	10	1.51906	1.86453	1.38639
	20	2.01763	2.04934	1.98292
	40	2.41566	2.49465	2.18525
	80	2.77624	2.78015	3.28464
809	5	1.42006	1.46684	1.44564
	10	1.93597	1.74022	1.7459
	20	1.90593	1.90286	1.8396
	40	2.5243	2.56928	2.28119
	80	2.85613	2.72446	2.72311
1009	5	1.533374	1.40633	1.4586
	10	1.8659	1.91756	1.9741
	20	1.98516	2.02909	2.08034
	40	2.34565	2.29367	2.48521
	80	3.06404	2.87213	3.08415

n	d	$r\ (\gamma_j = 1)$	$r\ (\gamma_j = 1/j^2)$	$r\ (\gamma_j = (0.5)^j)$
2003	5	1.76989	1.44861	1.55169
	10	2.16058	1.98488	2.10321
	20	2.00492	2.02555	2.05145
	40	2.46197	2.41568	2.42426
	80	3.01589	3.12879	2.72311
4001	5	1.73799	1.73593	1.67204
	10	2.03304	2.11947	2.13126
	20	2.29004	2.21185	2.28748
	40	2.85172	2.95931	2.82595
	80	3.23235	3.17223	3.26718
8009	5	1.84455	1.77299	1.73538
	10	1.933	1.94913	1.89745
	20	2.31343	2.38194	2.14583
	40	2.61951	2.46625	2.49397
	80	3.07129	3.13869	3.28764
16001	5	1.8236	1.75291	1.74923
	10	2.15757	2.0878	2.01515
	20	2.30053	2.32613	2.43989
	40	2.274121	2.71713	2.7027
	80	3.22472	3.04241	3.24138
32003	5	2.41275	2.03441	1.94906
	10	2.25323	2.15031	2.02382
	20	2.41239	2.39788	2.37847
	40	2.49959	2.90805	2.96568
	80	3.47078	3.22363	3.34058

6.6.3 Concluding remarks

The numerical experiments from the previous subsection suggest that shifted lattice rules in the unit cube have merit in approximating integrals over Euclidean space. Although the theoretical convergence error is $O(n^{-1/2})$, the numerical experiments suggest that in practice a better convergence rate could be obtained. A similar behaviour of the error has also been observed in [38] and [62].

Another observation is that if the weights are summable (these are typically the situations to be considered in practice), then an increase in the dimension will not dramatically decrease the precision for a fixed n. This situation corresponds to the concept of "limiting discrepancy" from [57]. In simple terms, such limiting discrepancy is defined as the limit when $d \to \infty$ from the discrepancy of the quadrature points. It has also been proved in [57] that the limiting discrepancy is finite if and only if the weights are summable.

Finally, let us remark that our first attempt was to obtain the results in this chapter under a more general weight setting (for instance the general weights used in [48] or Chapter 2) and when n is not necessarily prime. However under the assumptions within this chapter, it seems difficult to obtain such extensions. The same observation is also valid for the results obtained in [38] and [62]. In the next chapter however, we use the usual weighted star discrepancy as defined by (2.2) to obtain results for integrals over Euclidean space under a general weighted setting. Moreover, we also improve the theoretical convergence rate from $O(n^{-1/2})$ obtained here to a better $O(n^{-1+\delta})$ for any $\delta > 0$.

Chapter 7

Shifted lattice rules based on a general weighted discrepancy for integrals over Euclidean space

In this chapter we approximate weighted integrals over Euclidean space by using shifted rank-1 lattice rules having good bounds for the "generalised weighted star discrepancy". This version of the discrepancy corresponds to the classic L_∞ weighted star discrepancy via a mapping to the unit cube. Under a general weighted assumption (the same as in Chapter 2), we first show the existence of shifted lattice rules that have good bounds for the weighted star discrepancy by using an averaging argument. The component-by-component technique is used later to construct the generating vector of these shifted lattice rules. We prove that the bound on the generalised weighted star discrepancy considered here is of order $O(n^{-1+\delta})$ for any $\delta > 0$ and with the involved constant independent of the dimension. This convergence rate is better than the typical $O(n^{-1/2})$ achieved for Monte-Carlo methods as well as the theoretical convergence observed in Chapter 6.

7.1 Introduction

As in Chapter 6, we consider integrals given by (see also (1.4))

$$I_d(f,\rho) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

where $\rho(\boldsymbol{x})$ is a probability density function assumed to have the same product form as in Chapter 6, namely $\rho(\boldsymbol{x}) = \prod_{j=1}^{d}\rho_j(x_j)$, where each ρ_j is a probability density over $\mathbb{R}$. For simplicity we also assume that the 1-dimensional densities ρ_j are equal.

As we mentioned in the previous chapter, such integrals can be first transformed to equivalent integrals over the unit cube by using the mapping $u = \Phi(x) = \int_{-\infty}^{x}\rho(t)\,\mathrm{d}t, \forall x \in \mathbb{R}$ for each coordinate direction (see also (6.2)) and the transformed integrals can be approximated by constructing shifted lattice rules over the unit cube. Let us recall from Chapter 6 that these integrals become

$$I_d(f,\rho) = \int_{[0,1]^d} f(\Phi^{-1}(\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u} = \int_{[0,1]^d} g(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} := I_d(g),$$

where $g = f \circ \Phi^{-1}$ is applied component-wise. Integrals over the unit cube might be approximated by quadrature rules of the form

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

where $\boldsymbol{w}_k \in [0,1]^d$, for all $0 \le k \le n-1$ and $\boldsymbol{t}_k = \Phi^{-1}(\boldsymbol{w}_k) \in \mathbb{R}^d$ for all $0 \le k \le n-1$ with the inverse mapping Φ^{-1} applied component-wise.

In this chapter we are interested in constructing shifted rank-1 lattice rules suitable for integrals over Euclidean space by using a weighted star discrepancy as a criterion of goodness. Such shifted rank-1 lattice rules are of the form (recall also (1.6))

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

where $\boldsymbol{z}$ is the generating vector having all the components assumed to be relatively prime with n, while $\boldsymbol{\Delta} \in [0,1)^d$ is the shift. Shifted lattice rules suitable for integrals over unbounded regions have been previously constructed

in weighted reproducing kernel Hilbert spaces (see [38], [62] and Chapter 6), under the assumption that the weights have a product form (see (1.12)). The purpose of the present chapter is to construct shifted rank-1 lattice rules for integrals over Euclidean space in a general weighted setting. In Chapter 2 (see also [48]), we constructed rank-1 lattice rules having a low weighted star discrepancy with the weights being general and mentioned that the techniques therein could be used for weighted integrands over unbounded regions, however without effectively presenting such a construction.

In Chapter 6 as well as in [38] and [62], the resulting error had the theoretical order of magnitude of $O(n^{-1/2})$, which is the same as the typical convergence expected from a Monte Carlo method. As we shall see later, the weighted star discrepancy used here in order to assess the goodness of a shifted lattice rule of the form (1.6) will have a better convergence order than the convergence observed in Chapter 6, [38] and [62], although slightly worse than the convergence from Chapter 2. The convergence observed in this chapter is the optimal $O(n^{-1+\delta})$ for any $\delta > 0$ and with the involved constant independent of the dimension. As we mentioned in the previous chapter, this convergence rate has been also obtained in [23] where the authors used a similar discrepancy as the discrepancy defined below by (7.1). However in [23], no explicit construction was given and the weights were assumed to be product. In this chapter, we provide an explicit construction and moreover, we allow weights to be more general than the product weights used in the mentioned paper. We should also mention that the settings throughout this chapter are different from those in Chapter 6 in the sense that another measure of goodness is used to evaluate the merit of the shifted lattice rules constructed here.

Let us also remark that under a general weighted assumption, there are no results to date in the specialised literature regarding construction of lattice rules suitable for integrals over unbounded regions, so we also fill a gap in this sense.

7.2 Generalised weighted star discrepancy

Since the weighted star discrepancy used earlier in Chapters 2–5 (see (2.2), (3.2) and (5.1)) was used to measure the goodness of lattice rules for integrals over the unit cube while here we want to approximate integrals over Euclidean space, it seems natural to introduce a measure of discrepancy of point sets taken from the whole Euclidean space. Let's recall first that the usual weighted star discrepancy of a point set P_n in the unit cube was defined in Chapter 2 by (see also (2.2)):

$$D^*_{n,\boldsymbol{\gamma}}(P_n) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} \left|\mathrm{discr}((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_n)\right|.$$

The "generalised weighted star discrepancy" considered in this chapter and defined below, will be obtained by using the inverse mapping Φ^{-1} (see also the transformation (6.2)) applied component-wise to the usual weighted star discrepancy. However, we remark that the concept of "generalised discrepancy" may be introduced not necessarily in connection with a mapping of the form (6.2).

Let's consider now an arbitrary point $\boldsymbol{y} = (y_1, y_2, \ldots, y_d)$ from $\mathbb{R}^d$ and denote $Y := (-\infty, y_1) \times (-\infty, y_2) \times \cdots \times (-\infty, y_d)$. The "generalised local star discrepancy" is then defined as follows:

Definition 7.1 *If W_n is a set of n distinct points from $\mathbb{R}^d$, $\boldsymbol{y}$ is an arbitrary point from $\mathbb{R}^d$ and ρ is a probability density function, then the generalised local star discrepancy at $\boldsymbol{y}$ is defined by:*

$$\mathrm{gdiscr}(\boldsymbol{y}, W_n) := \frac{|Y \cap W_n|}{n} - \int_Y \rho(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t}.$$

This definition corresponds to the definition of the local star discrepancy of points in the unit cube (see Definition 1.4). Next, corresponding to the concept of unweighted star discrepancy (see Definition 1.5), we can introduce the "generalised unweighted star discrepancy" as follows:

Definition 7.2 *The generalised unweighted star discrepancy is defined by*

$$GD^*_\rho(W_n) := \sup_{\boldsymbol{y}\in\mathbb{R}^d} \left|\mathrm{gdiscr}(\boldsymbol{y}, W_n)\right|.$$

Let's remark that this generalised discrepancy is related to the discrepancies used in [15], [16] and [23].

Let now $\boldsymbol{\gamma}_{\mathfrak{u}}$ be the weights associated with an arbitrary non-empty subset $\mathfrak{u}$ of $\mathcal{D} = \{1, 2, \ldots, d-1, d\}$ and let's denote by $\boldsymbol{y}_{\mathfrak{u}}$ the vector from $\mathbb{R}^{|\mathfrak{u}|}$ consisting of the components of $\boldsymbol{y}$ that belong to $\mathfrak{u}$. We also denote by $W_{n,\mathfrak{u}}$ the set obtained from the points of W_n by taking only the coordinates that belong to $\mathfrak{u}$ and make the convention that $W_{n,\mathcal{D}} = W_n$. With these notations, the generalised weighted star discrepancy can be defined by

$$GD^*_{n,\boldsymbol{\gamma}}(W_n) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sup_{\boldsymbol{y}_{\mathfrak{u}}\in\mathbb{R}^{|\mathfrak{u}|}} |\mathrm{gdiscr}(\boldsymbol{y}_{\mathfrak{u}}, W_{n,\mathfrak{u}})|\,. \tag{7.1}$$

As mentioned earlier, by using the transformation (6.2) component-wise, the generalised weighted star discrepancy defined by (7.1) corresponds to the usual weighted star discrepancy. Since $GD^*_{n,\boldsymbol{\gamma}}(W_n) = D^*_{n,\boldsymbol{\gamma}}(P_n)$, we can establish bounds on the generalised weighted star discrepancy by finding bounds on the usual weighted star discrepancy defined by (2.2). We can now apply the techniques on the unit cube (details can be found in [48] and in Chapter 2) to deduce that

$$|Q_{n,d}(g) - I_d(g)| \le D^*_{n,\boldsymbol{\gamma}}(P_n) \times \left(\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_{\mathfrak{u}}} g((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1})) \right| \mathrm{d}\boldsymbol{x}_{\mathfrak{u}} \right).$$

As in Chapter 2 (see also [48]), we shall also assume that the weight associated with a set should not be bigger than the weights associated with any of its subsets. Hence, for any non-empty subset $\mathfrak{u} \subseteq \mathcal{D}$, recall from (2.3) that

$$\boldsymbol{\gamma}_{\mathfrak{u}} \le \boldsymbol{\gamma}_{\mathfrak{g}} \quad \text{for any} \quad \mathfrak{g} \subseteq \mathfrak{u}.$$

In the next section we obtain bounds on the generalised weighted star discrepancy, while in Section 7.4 we prove that the generating vector for a shifted rank-1 lattice rules having good bounds for the generalised weighted star discrepancy can be constructed by using the usual component-by-component technique.

7.3 Bounds on the generalised weighted star discrepancy

For the rest of the chapter, we assume that $P_n = \{\{k\boldsymbol{z}/n + \boldsymbol{\Delta}\}, 0 \le k \le n-1\}$, where the components of the shift $\boldsymbol{\Delta}$ are of the form $\Delta_j = c_j/\ell$ with ℓ and c_j being positive integers. If we denote $N = \mathrm{lcm}(n, \ell)$, we see that the quadrature points in our shifted lattice rule can be rewritten as the fractional parts of

$$\frac{k\boldsymbol{z}}{n} + \frac{\boldsymbol{c}}{\ell} = \frac{k(N/n)\boldsymbol{z} + (N/\ell)\boldsymbol{c}}{N}.$$

At this point, we remark that the results that follow allow the shift to be chosen randomly, provided the components are rational numbers. This requirement comes from the fact that some of the Niederreiter's results from [42] (see also Theorem 2.2 and Theorem 2.3) that will be used next (for instance to obtain (7.2)) are applicable only for vectors having rational components. We also mention that in [52], shifted lattice rules have been previously constructed with the components of $\boldsymbol{c}$ taken from the set $\{1, 3, \ldots, 2n-1\}$, while $\ell = 2n$. We could choose a similar form for the shift here, however we prefer to allow slightly more generality. Nevertheless, we still require that ℓ be chosen such that $m = N/n$ is an integer independent of d and n.

It then follows from Theorem 2.2 that

$$\begin{aligned} &\sup_{\boldsymbol{x}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} |\mathrm{discr}\,((\boldsymbol{x}_{\mathfrak{u}}, \mathbf{1}), P_n)| \qquad (7.2)\\ \le\ & 1 - (1-1/N)^{|\mathfrak{u}|} + \sum_{\boldsymbol{h} \in E^*_{N,|\mathfrak{u}|}} \frac{1}{\prod_{j \in \mathfrak{u}} r(h_j, N)} \left| \frac{1}{n} \sum_{k=0}^{n-1} e^{2\pi \mathrm{i} \boldsymbol{h} \cdot (k(N/n)\boldsymbol{z}_{\mathfrak{u}} + (N/\ell)\boldsymbol{c}_{\mathfrak{u}})/N} \right|, \end{aligned}$$

where $E^*_{n,m}$ was defined in Chapter 2 (see (2.8)), while we recall that

$$r(h, M) = \begin{cases} M \sin(\pi |h|/M), & \text{if } h \ne 0\ , \\ 1, & \text{otherwise.} \end{cases}$$

Obviously, $\boldsymbol{z}_{\mathfrak{u}}$ and $\boldsymbol{c}_{\mathfrak{u}}$ are the vectors consisting of the components of $\boldsymbol{z}$ and $\boldsymbol{c}$,

respectively, whose indices belong to $\mathfrak{u}$. Now we have

$$\begin{aligned}\left|\frac{1}{n}\sum_{k=0}^{n-1} e^{2\pi \mathrm{i}\boldsymbol{h}\cdot(k(N/n)\boldsymbol{z}_{\mathfrak{u}}+(N/\ell)\boldsymbol{c}_{\mathfrak{u}})/N}\right| &= \left|\frac{1}{n}\sum_{k=0}^{n-1} e^{2\pi \mathrm{i}k\boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{u}}/n}\right| \left|e^{2\pi \mathrm{i}\boldsymbol{h}\cdot\boldsymbol{c}_{\mathfrak{u}}/\ell}\right| \\ &= \begin{cases} 1, & \text{if } \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{u}} \equiv 0 \,(\mathrm{mod}\, n)\,, \\ 0, & \text{if } \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{u}} \not\equiv 0 \,(\mathrm{mod}\, n)\,. \end{cases}\end{aligned}$$

In the last step we used the obvious equality $\left|e^{2\pi \mathrm{i}\boldsymbol{h}\cdot\boldsymbol{c}_{\mathfrak{u}}/\ell}\right| = 1$. Since $\sin(\pi t) \geq 2t$ for $0 \leq t \leq 1/2$, then from (7.2) and Theorem 2.3, it follows that

$$\sup_{\boldsymbol{x}_{\mathfrak{u}}\in[0,1]^{|\mathfrak{u}|}} |\mathrm{discr}\,((\boldsymbol{x}_{\mathfrak{u}},\mathbf{1}),P_n)| \leq 1-(1-1/N)^{|\mathfrak{u}|}+\frac{1}{2}R_N(\boldsymbol{z},\mathfrak{u})\,,$$

where (see also the arguments that lead to (2.10) in Chapter 2)

$$\begin{aligned}R_N(\boldsymbol{z},\mathfrak{u}) &= \sum_{\substack{\boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{u}}\equiv 0\,(\mathrm{mod}\ n)\\ \boldsymbol{h}\in E^*_{N,|\mathfrak{u}|}}} \prod_{j\in\mathfrak{u}} \frac{1}{\max(1,|h_j|)} \\ &= \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}\left(1+\sum_{-N/2<h\leq N/2}{}' \frac{e^{2\pi \mathrm{i}hkz_j/n}}{|h|}\right)-1.\end{aligned}$$

Since the point set P_n depends actually on the vector $\boldsymbol{z}$, we shall denote the discrepancy $D^*_{n,\boldsymbol{\gamma}}(P_n)$ by $D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z})$. Of course, the notation $GD^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z})$ could be used for the generalised weighted star discrepancy given by (7.1), since each point in W_n is obtained by applying the inverse mapping Φ^{-1} to a point in P_n. Clearly, we now have

$$GD^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}\left(1-(1-1/N)^{|\mathfrak{u}|}+\frac{1}{2}R_N(\boldsymbol{z},\mathfrak{u})\right). \tag{7.3}$$

From (2.13) (see Chapter 2), we obtain

$$\max_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}}\left(1-(1-1/N)^{|\mathfrak{u}|}\right) \leq \frac{1}{N}\max_{\mathfrak{u}\subseteq\mathcal{D}} |\mathfrak{u}|\boldsymbol{\gamma}_{\mathfrak{u}}. \tag{7.4}$$

Also in Chapter 2, it was established that

$$R_N(\boldsymbol{z},\mathfrak{u}) = \sum_{\mathfrak{g}\subseteq\mathfrak{u}} \widetilde{R}_N(\boldsymbol{z},\mathfrak{g}),$$

where (see also (2.15) and (2.17))

$$\widetilde{R}_N(\boldsymbol{z},\mathfrak{g}) = \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{g}}\left(\sum_{-N/2<h\leq N/2}{}' \frac{e^{2\pi \mathrm{i}hkz_j/n}}{|h|}\right) = \sum_{\substack{\boldsymbol{h}\in\widetilde{E}^*_{N,|\mathfrak{g}|}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{g}}\equiv 0\,(\mathrm{mod}\ n)}} \prod_{j\in\mathfrak{g}}\frac{1}{|h_j|} \geq 0,$$

with $\widetilde{E}^*_{n,m}$ as introduced by (2.16). From the inequality (2.18) and by using (7.3) and (7.4) (see also the arguments leading to Lemma 2.4), we obtain

$$D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \frac{1}{N} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2} e^2_{n,d}(\boldsymbol{z}),$$

where here

$$e^2_{n,d}(\boldsymbol{z}) := \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}).$$

For the rest of the chapter we shall assume that n prime. In this case, bounds on $e^2_{n,d}(\boldsymbol{z})$ can be obtained by finding an expression for a certain mean value of $e^2_{n,d}(\boldsymbol{z})$. The mean is taken over all integer vectors $\boldsymbol{z} \in \mathcal{Z}_n^d$, where $\mathcal{Z}_n = \{1, 2, \ldots, n-1\}$ and is, as usual in the prime case, defined by

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} e^2_{n,d}(\boldsymbol{z}).$$

An expression for the mean is given in the next theorem.

Theorem 7.1 *Let n be prime. Then*

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} + \frac{n-1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|},$$

where we recall that

$$S_n = \sum_{-n/2 < h \le n/2}{}' \frac{1}{|h|}.$$

Proof. The proof follows the same ideas as in the proof of Theorem 2.6. Thus, from the definition of the mean, (2.15) and (2.19), we have

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-N/2 < h \le N/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right) \right).$$

By separating out the $k = 0$ term, we obtain

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} + \Theta_{N,d,\boldsymbol{\gamma}}, \tag{7.5}$$

where

$$\begin{aligned} \Theta_{N,d,\boldsymbol{\gamma}} &= \frac{1}{(n-1)^d} \sum_{\boldsymbol{z} \in \mathcal{Z}_n^d} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\frac{1}{n} \sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-N/2 < h \le N/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right) \right) \\ &= \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\sum_{k=1}^{n-1} \prod_{j \in \mathfrak{u}} \left(\frac{1}{n-1} \sum_{z_j=1}^{n-1} \sum_{-N/2 < h \le N/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right) \right). \end{aligned}$$

For every $1 \leq k \leq n-1$, consider now

$$T_N(k) = \frac{1}{n-1} \sum_{z_j=1}^{n-1} \sum_{-\frac{N}{2}<h\leq\frac{N}{2}}{}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|},$$

which is actually the quantity (2.20) defined in Chapter 2. Hence, by using Lemma 2.5, it follows that (see also (2.21))

$$T_N(k) = \frac{S_{N/n} - S_N}{n-1}.$$

This leads to

$$\Theta_{N,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{k=1}^{n-1} \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|} = \frac{n-1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|}.$$

Replacing now the last term in (7.5) with this expression, we obtain the desired result. □

Corollary 7.2 *Let n be prime. Then there exists a generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$e_{n,d}^2(\boldsymbol{z}) \leq M_{N,d,\boldsymbol{\gamma}} \leq \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}.$$

Proof. The first inequality is trivial. To obtain the second inequality, we observe first that the mean can be written as

$$M_{N,d,\boldsymbol{\gamma}} = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(S_N^{|\mathfrak{u}|} + (n-1) \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|} \right).$$

If $|\mathfrak{u}|$ is odd, then $S_{N/n} - S_N \leq 0$ and the expression in the outer brackets will be bounded by $S_N^{|\mathfrak{u}|}$. If $|\mathfrak{u}|$ is even, then $|\mathfrak{u}| \geq 2$ and it follows that

$$(n-1) \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|} \leq (n-1) \frac{S_N^{|\mathfrak{u}|}}{(n-1)^2} = \frac{S_N^{|\mathfrak{u}|}}{n-1}.$$

So regardless whether $|\mathfrak{u}|$ is odd or even, it follows that

$$S_N^{|\mathfrak{u}|} + (n-1) \left(\frac{S_{N/n} - S_N}{n-1} \right)^{|\mathfrak{u}|} \leq S_N^{|\mathfrak{u}|} + \frac{S_N^{|\mathfrak{u}|}}{n-1},$$

which leads to

$$M_{N,d,\boldsymbol{\gamma}} \leq \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \left(S_N^{|\mathfrak{u}|} + \frac{S_N^{|\mathfrak{u}|}}{n-1} \right) \leq \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}.$$

This completes the proof. □

From this corollary, we can now obtain:

Corollary 7.3 *Suppose the weights satisfy* (2.3) *and suppose that n is prime. Then there exists a vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that the generalised weighted star discrepancy satisfies the bound*

$$GD^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \frac{1}{N} \max_{\mathfrak{u} \subseteq \mathcal{D}} |\mathfrak{u}| \boldsymbol{\gamma}_{\mathfrak{u}} + \frac{1}{2(n-1)} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}. \tag{7.6}$$

From Chapter 2 or [48], it will follow that the bound given by (7.6) has the order of magnitude of $O(n^{-1}(\ln N)^d)$, with the involved constant depending on d. Recalling that $m = N/n$ is independent of n, we see that the bound is actually of order $O(n^{-1}(\ln n)^d)$, with the constant depending on d and m. Such a bound is slightly worse than the bound for the discrepancy in Chapter 2, but we still can obtain strong tractability under further assumptions over the weights. Indeed, if we assume that the weights are such that (2.3) is satisfied and

$$\sum_{\mathfrak{u} \subseteq \mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} \le C(\boldsymbol{\gamma}, \delta, m) n^{\delta},$$

for some $\delta > 0$, where $C(\boldsymbol{\gamma}, \delta, m)$ is independent of d and n, then for any prime n, we see from (7.6) there exists a generating vector $\boldsymbol{z}$ (in the next section we prove that the CBC algorithm yields such a $\boldsymbol{z}$), for which the generalised weighted discrepancy and the corresponding weighted discrepancy satisfy the strong tractability error bound

$$GD^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) = D^*_{n,\boldsymbol{\gamma}}(\boldsymbol{z}) \le 2C(\boldsymbol{\gamma}, \delta, m) n^{-1+\delta},$$

with the involved constant depending on the weights, δ and m, but independent of the dimension. An example of weights $\boldsymbol{\gamma}_{\mathfrak{u}}$ having this property is when the weights $\boldsymbol{\gamma}_{\mathfrak{u}}$ are product and the γ_j are summable. A full proof of such a result is given in Theorem 3.4 and further details may also be found in [20] and [29].

We conclude this section by mentioning that the bound of magnitude $O(n^{-1+\delta})$ for any $\delta > 0$ obtained here is better than the typical bound of order $O(n^{-1/2})$ yielded by Monte Carlo methods or the same $O(n^{-1/2})$ attained in

Chapter 6. However in Chapter 6, as well as in [38] and [62], a different measure of goodness was used. The convergence obtained in this chapter is likely to be the best convergence rate one could expect. Thus, we have established that the generalised weighted star discrepancy can be used as a viable criterion of goodness for the approximation of weighted integrals over $\mathbb{R}^d$. Moreover, the results here can be used for general weight settings, not only in the context of product weights.

7.4 Component-by-component construction of the generating vector

Component-by-component algorithm

1. Set the value for the first component of the vector, say $z_1 = 1$.

2. For $m = 2, 3, \ldots, d$, find $z_m \in \mathcal{Z}_n$ such that $e^2_{n,m}(z_1, \ldots, z_m)$ is minimised. Here

$$e^2_{n,m}(z_1, \ldots, z_m) = \sum_{\mathfrak{u} \subseteq \{1,2,\ldots,m\}} \gamma_{\mathfrak{u}} \widetilde{R}_N((z_1, \ldots, z_m), \mathfrak{u}).$$

Now we prove that the algorithm does indeed yield good shifted rank-1 lattice rules. By good, we mean that the $\boldsymbol{z}$ found this way satisfies the bound for $e^2_{n,d}(\boldsymbol{z})$ given in Corollary 7.2.

Theorem 7.4 *Let n be prime. Suppose there exists a $\boldsymbol{z} \in \mathcal{Z}_n^d$ such that*

$$e^2_{n,d}(\boldsymbol{z}) \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} S_N^{|\mathfrak{u}|}. \tag{7.7}$$

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

$$e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \le \frac{1}{n-1} \sum_{\mathfrak{u} \subseteq \mathcal{D}_1} \gamma_{\mathfrak{u}} S_N^{|\mathfrak{u}|},$$

where $\mathcal{D}_1 = \mathcal{D} \cup \{d+1\}$. Such a z_{d+1} can be found by minimising $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over the set $\mathcal{Z}_n$.

Proof. We have

$$\begin{aligned} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) &= \sum_{\mathfrak{u}\subseteq\mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_N((\boldsymbol{z}, z_{d+1}), \mathfrak{u}) \\ &= \sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}) + \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \widetilde{R}_N((\boldsymbol{z}, z_{d+1}), \mathfrak{u}). \end{aligned} \tag{7.8}$$

In a similar way as in Chapter 2, we define

$$C_k(z) = \sum_{-N/2<h\le N/2}{}' \frac{e^{2\pi \mathrm{i} hkz/n}}{|h|}, \quad 0 \le k \le n-1.$$

It is easy to see that $C_0(z) = S_N$. Using (2.15), for $\mathfrak{u} \subseteq \mathcal{D}_1$ with $d+1 \in \mathfrak{u}$ and by separating out the $k = 0$ term, we obtain

$$\widetilde{R}_N((\boldsymbol{z}, z_{d+1}), \mathfrak{u}) = \frac{S_N^{|\mathfrak{u}|}}{n} + \frac{1}{n}\sum_{k=1}^{n-1} \left(\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) \right) C_k(z_{d+1}).$$

Substituting this in (7.8), we obtain

$$\begin{aligned} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) &= e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} \\ &\quad + \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \frac{\boldsymbol{\gamma}_{\mathfrak{u}}}{n} \sum_{k=1}^{n-1} \left(\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) \right) C_k(z_{d+1}). \end{aligned}$$

Next we average $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over all possible values of $z_{d+1} \in \mathcal{Z}_n$ and consider

$$\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) = \frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}).$$

As the dependency of $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ on z_{d+1} is only through the $C_k(z_{d+1})$ factor, we next focus on the quantity

$$\frac{1}{n-1} \sum_{z_{d+1}=1}^{n-1} C_k(z_{d+1}),$$

which actually is the quantity $T_N(k)$ introduced by (2.20). Using now (2.21), we obtain

$$\begin{aligned} &\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \\ = \; & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} - \frac{S_N - S_{N/n}}{n(n-1)} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} \sum_{k=1}^{n-1} \prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j). \end{aligned}$$

For any $\mathfrak{u} \subseteq \mathcal{D}_1$ with $d+1 \in \mathfrak{u}$, we have

$$-\frac{1}{n}\sum_{k=1}^{n-1}\prod_{j\in\mathfrak{u}-\{d+1\}} C_k(z_j) = -\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}-\{d+1\}) + \frac{S_N^{|\mathfrak{u}|-1}}{n} \leq \frac{S_N^{|\mathfrak{u}|-1}}{n},$$

where we have subtracted and added the $k=0$ term and used the fact that the quantities $\widetilde{R}_N(\boldsymbol{z}, \mathfrak{g})$ are positive for any subset $\mathfrak{g} \subseteq \mathcal{D}$. Using also the inequality $S_N - S_{N/n} \leq S_N$, we obtain

$$\begin{aligned}
& \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \\
\leq\ & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n}\sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} + \frac{S_N - S_{N/n}}{n(n-1)} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|-1} \\
\leq\ & e^2_{n,d}(\boldsymbol{z}) + \frac{1}{n-1}\sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}.
\end{aligned}$$

From the hypothesis, we next deduce that

$$\begin{aligned}
\mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})) \ &\leq\ \frac{1}{n-1}\sum_{\mathfrak{u}\subseteq\mathcal{D}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} + \frac{1}{n-1}\sum_{\substack{\mathfrak{u}\subseteq\mathcal{D}_1 \\ d+1\in\mathfrak{u}}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|} \\
&=\ \frac{1}{n-1}\sum_{\mathfrak{u}\subseteq\mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}. \qquad (7.9)
\end{aligned}$$

There must be at least one $z_{d+1} \in \mathcal{Z}_n$ such that $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \leq \mathrm{Avg}(e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}))$ and this z_{d+1} may be chosen by minimising $e^2_{n,d+1}(\boldsymbol{z}, z_{d+1})$ over the set $\mathcal{Z}_n$. From (7.9), it is clear now that for the chosen z_{d+1}, we have

$$e^2_{n,d+1}(\boldsymbol{z}, z_{d+1}) \leq \frac{1}{n-1}\sum_{\mathfrak{u}\subseteq\mathcal{D}_1} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|},$$

which is the desired result. □

From this theorem we can deduce the following:

Corollary 7.5 *Let n be prime. Then for $1 \leq m \leq d$ we can construct a vector $\boldsymbol{z} \in \mathcal{Z}_n^m$ such that*

$$e^2_{n,m}(z_1, \ldots, z_m) \leq \frac{1}{n-1}\sum_{\mathfrak{u}\subseteq\{1,2,\ldots,m\}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}.$$

We can set $z_1 = 1$ and for $2 \leq m \leq d$, every z_m can be found by minimising $e^2_{n,m}(z_1, \ldots, z_m)$ over the set $\mathcal{Z}_n$.

Proof. In the case $d = 1$, it is easy to verify using the expression for the mean that $M_{N,1,\{\gamma_{\{1\}}\}} = \frac{\gamma_{\{1\}} S_{N/n}}{n}$. This is to be expected since it is also relatively easy to verify by using (2.15) that $\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}) = \frac{S_{N/n}}{n}$ whenever $|\mathfrak{u}| = 1$. Indeed, in such a case we have

$$\begin{aligned}\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}) &= \frac{1}{n} \sum_{k=0}^{n-1} {\sum_{-N/2<h\leq N/2}}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \left({\sum_{\substack{-N/2<h\leq N/2 \\ h\equiv 0 \,(\bmod\, n)}}}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} + {\sum_{\substack{-N/2<h\leq N/2 \\ h\not\equiv 0 \,(\bmod\, n)}}}' \frac{e^{2\pi \mathrm{i} h k z_j/n}}{|h|} \right).\end{aligned}$$

Using next similar arguments as in the proof of Lemma 2.5 (see also the proof of Corollary 3.6), it follows that $\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u}) = \frac{S_{N/n}}{n}$, which leads to $e^2_{n,1}(z) = \frac{\gamma_{\{1\}} S_{N/n}}{n}$ for any $z \in \mathcal{Z}_n$. So, the inequality (7.7) holds for $d = 1$ and the whole result then follows immediately from Theorem 7.4. □

Special classes of general weights are the so-called "order-dependent" and "finite-order" weights, which lead to a significant reduction of the computational costs incurred by the construction. These weights were defined in Chapter 2 by Definition 2.2 and Definition 2.3. Let us also recall that Section 2.5 (see also [48]) was dedicated to the CBC construction for these particular classes of weights. Similar results will hold here as a consequence from Theorem 7.4 and Corollary 7.5 and these results are presented below.

Let's denote by Γ_i the weight associated with a set containing i elements for $1 \leq i \leq d$. Now, by taking $\boldsymbol{\gamma}_{\mathfrak{u}} = \Gamma_i$ whenever $|\mathfrak{u}| = i$ and noting that the number of subsets of $\mathcal{D}$ with i elements is $\binom{d}{i}$, we obtain that for order-dependent weights, the generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that

$$e^2_{n,d}(\boldsymbol{z}) \leq \frac{1}{n-1} \sum_{i=1}^{d} \Gamma_i \binom{d}{i} S_N^i.$$

If the weights are finite-order, the generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that

$$e^2_{n,d}(\boldsymbol{z}) \leq \frac{1}{n-1} \sum_{\substack{\mathfrak{u}\subseteq\mathcal{D} \\ |\mathfrak{u}|\leq q^*}} \boldsymbol{\gamma}_{\mathfrak{u}} S_N^{|\mathfrak{u}|}.$$

If the weights are both order-dependent and finite-order, the generating vector $\boldsymbol{z} \in \mathcal{Z}_n^d$ may be constructed component-by-component such that

$$e_{n,d}^2(\boldsymbol{z}) \leq \frac{1}{n-1} \sum_{\ell=1}^{q^*} \Gamma_i \binom{d}{i} S_N^i.$$

The costs incurred by the CBC construction were analysed in depth in Section 2.7 and [48] and a similar analysis can be used here with a few minor modifications. Let's observe first that from (2.15), it follows that the cost of calculating each $\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u})$ is $O\left(Nn|\mathfrak{u}|\right)$ operations. However, it is shown in Appendix A (see also [31], [29, Appendix A] and Chapter 3) that this cost can be reduced at the expense of extra storage. Recall that such a reduction of cost is based on the fact that the quantities of the form

$$\sum_{-N/2<h\leq N/2}{}' \frac{e^{2\pi \mathrm{i} hq/n}}{|h|}, \quad 0 \leq q \leq n-1, \tag{7.10}$$

used in the expression for $\widetilde{R}_N(\boldsymbol{z}, \mathfrak{u})$, can be computed in $O(N)$ operations and then stored.

Similar costs as in Chapter 2 will then follow, the main difference being the additional number of operations needed to compute each quantity given by (7.10). Since $N = nm$ and m is fixed, we have $N = O(n)$. In conclusion, the total cost of the construction is at most $O(n^2 d 2^d)$ and the cost becomes $O(n^2 d^{q^*+1})$ for finite-order weights, $O(n^2 d^2)$ for order-dependent weights, and $O(n^2 d q^*)$ for weights that are both finite-order and order-dependent plus additional storage. Let us finally remark that the fast CBC construction (see [6, Section 4] and [44] for details) can also be used here in the same way as in Chapter 2. Thus, the total maximum of $O(n^2 d 2^d)$ operation count may be reduced to $O(n \ln(n) d 2^d)$, while for finite-order weights the operation count may be reduced to $O(n \ln(n) d^{q^*+1})$. In each situation we also need to add the amount required for storage. In the case of order-dependent weights, the total operation count may actually be reduced to $O(nd \ln(n) + nd^2)$ with $O(nd)$ additional storage, while if the weights are both order-dependent and finite-order, then the cost of the construction will be $O(nd \ln(n) + ndq^*)$ with $O(nq^*)$ additional storage.

Chapter 8

Conclusion

In this thesis, we established theoretical results on the construction of lattice rules for multiple integration based on a low weighted discrepancy. For the unweighted discrepancy, theoretical results were previously known from works such as [42] and [51] where it was established that the best order of magnitude for the discrepancy is $O(n^{-1}(\ln\ n)^d)$, with the involved constant depending on the dimension d. When d is large, then a huge number of points is required for reasonable accuracy, and this makes quasi-Monte Carlo methods impractical (the "curse of dimensionality"). In a weighted setting, the existing theoretical background was developed mainly by assuming that integrands belong to certain reproducing kernel Hilbert spaces and by using an L_2 version of the weighted star discrepancy as a criterion of goodness.

We reinforce that the construction of lattice rules depends on the criterion of goodness chosen as well as on the weight settings and the type of lattice rule considered; it depends on whether the number of points is prime or not; and it also depends on whether the domain is bounded or not. Despite the known theoretical background, we should mention that a whole separate analysis is required for every particular assumption made together with the development of the underlying theory. In this sense, the thesis fills several gaps and some of the advantages of the techniques used here were mentioned in the first chapter. More important, the theory developed here leads to construction

algorithms and, it is hoped that future research will prove the usefulness of such algorithms in practical applications. Overall, we have shown that under appropriate conditions over the weights, we can construct lattice rules so that the order of magnitude of the corresponding quadrature error ranges from $O(n^{-1/2})$ to $O(n^{-1+\delta})$ for any $\delta > 0$ and, moreover, the involved constant is independent of the dimension.

From the theoretical point of view, we believe that the results obtained here could further be refined. For instance, it would be interesting to see whether lattice rules with a non-prime number of points could be constructed under a general weighted setting and maybe then extended to lattice rules suitable for integrals over Euclidean space. It would also be of interest to improve the theoretical convergence of $O(n^{-1/2})$ obtained in Chapter 6. Finally, maybe further theoretical results on the generalised weighted discrepancy from Chapter 7 could be developed in the future. Thus, the whole thesis not only establishes new results on the construction of lattice rules, but also indicates a path to future research.

Appendix A

Let n and m be integers so that m is fixed and let's denote $N = nm$. In this appendix, we show that the values of $F_N(q/n)$ for $0 \leq q \leq n-1$, where

$$F_N(x) = \sum_{-N/2<h\leq N/2}{}' \frac{e^{2\pi \mathrm{i} hx}}{|h|}, \quad 0 \leq x \leq 1,$$

can be calculated at a total cost of $O(N)$ operations.

It is easy to see that $F_N(x) = F_N(1-x)$, so it will suffice to consider $0 \leq x \leq \frac{1}{2}$. Accordingly, we will need to calculate at most $\lfloor n/2 \rfloor + 1$ values of the form $F_N(q/n)$. Let us remark that the results in [31] were developed in the situation when $N = n$, but they can be extended to the situation when $N \neq n$ by using the same techniques. For completeness, we present the main ideas below.

First we observe that when N is odd then

$$F_N(x) = 2 \sum_{h=1}^{(N-1)/2} \frac{\cos(2\pi hx)}{h},$$

while when N is even we have

$$F_N(x) = \frac{2e^{\pi \mathrm{i} Nx}}{N} + 2 \sum_{h=1}^{(N-2)/2} \frac{\cos(2\pi hx)}{h}.$$

Let us consider now

$$S(x, \eta) = \sum_{h=1}^{\eta-1} \frac{\cos(2\pi hx)}{h},$$

where

$$\eta(N) = \begin{cases} \frac{N+1}{2}, & N \text{ odd}, \\ \frac{N}{2}, & N \text{ even}. \end{cases}$$

From [31], it follows that

$$S(x, \eta) = \sum_{h=1}^{\infty} \frac{\cos(2\pi hx)}{h} - H(x, \eta) = -\ln(2\sin(\pi x)) - H(x, \eta),$$

where

$$H(x,\eta)=\sum_{h=\eta}^{\infty}\frac{\cos(2\pi hx)}{h}.$$

According to [31], $H(x,\eta)$ can be approximated by

$$H_T(x,\eta)=\sum_{k=0}^{T}b_k(x,\eta)\cos\left[\pi\left((2\eta+k-1)x+\frac{k+1}{2}\right)\right],$$

where

$$b_k(x,\eta)=\frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(2\sin(\pi x))^{k+1}}.$$

Consider now the approximation

$$F_{N,T}(x)=\begin{cases}-2\ln(2\sin(\pi x))-2H_T(x,\eta(N)), & N \text{ odd},\\ \frac{2e^{\pi iNx}}{N}-2\ln(2\sin(\pi x))-2H_T(x,\eta(N)), & N \text{ even},\end{cases}$$

Then we can establish a similar result with a similar proof as [31, Theorem 4]:

Theorem A.1 *Let $\varepsilon>0$ be given and $n\geq 5$ be a given integer such that $N=nm$, with m a fixed integer independent of n. Consider also the positive integers α and T satisfying the following conditions: $2\leq\alpha\leq\sqrt[3]{6n^2/\pi^2}$, and*

$$\frac{4(T+1)!}{(m(\alpha-1)\pi)^{T+2}}\leq\varepsilon.$$

If $F_N(x)$ is approximated by $F_{N,T}(x)$ for $\alpha/n\leq x\leq 1/2$, then

$$|F_N(x)-F_{N,T}(x)|\leq\varepsilon.$$

Proof. From the proof of [31, Theorem 4], it will follow first that

$$2\sin(\pi x)\geq 2\frac{(\alpha-1)\pi}{n},$$

and

$$|F_N(x)-F_{N,T}(x)|\leq\frac{4(T+1)!}{(2\sin(\pi x))^{T+2}\eta(\eta+1)\cdots(\eta+T+1)}.$$

From the hypothesis and using that $\eta(N)\geq N/2$, we next obtain

$$\begin{aligned}|F_N(x)-F_{N,T}(x)| &\leq \left(\frac{n}{2(\alpha-1)\pi}\right)^{T+2}\frac{4(T+1)!}{\eta(\eta+1)\cdots(\eta+T+1)}\\ &\leq \left(\frac{n}{2(\alpha-1)\pi}\right)^{T+2}\frac{4(T+1)!}{\left(\frac{N}{2}\right)^{T+2}}\\ &= \frac{4(T+1)!}{(m(\alpha-1)\pi)^{T+2}}\leq\varepsilon.\end{aligned}$$

□

Thus, the explicit formula for F_N is used at most α times when $0 \leq x < \alpha/n$, while the approximation $F_{N,T}$ is by the other hand used at most $\lfloor n/2 \rfloor - \alpha + 1$ times. This indicates that the total amount of operations required to compute all the quantities $F_N(q/n), 0 \leq q \leq n-1$, would be $O(N\alpha) + O(T(\lfloor n/2 \rfloor - \alpha + 1)) = O(N)$. These quantities can then be stored in $O(n)$ memory locations.

As an example, if we assume that $n \geq 100$ and $m = 3$ and we want to calculate F_N with an accuracy of $\varepsilon = 10^{-20}$, it turns that $\alpha = 18$ and $T = 12$. As another example, if we want a precision of $\varepsilon = 10^{-17}$, then for $n \geq 180$ and $m = 1$ (in this case $N = n$), we can take $\alpha = 27$ and $T = 13$.

Appendix B

Let us first recall that Lemma 6.5 was given in Chapter 6 as follows:

Lemma 6.5 *The function* $\psi(w) = \int_0^1 \mathcal{K}(\{w+\Delta\}, \Delta)\,\mathrm{d}\Delta$ *can be written as*

$$\psi(w) = 2\psi_1(w) + 2\psi_1(1-w), \quad \forall w \in (0,1),$$

where

$$\psi_1(w) = \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w+\Phi(t)), t)\rho(t)\,\mathrm{d}t.$$

Proof. From the expression of ψ, it is easy to see that we can write

$$\psi(w) = \int_0^{1-w} \mathcal{K}(w+\Delta, \Delta)\,\mathrm{d}\Delta + \int_{1-w}^1 \mathcal{K}(w+\Delta-1, \Delta)\,\mathrm{d}\Delta.$$

Following now an idea from [62], we split ψ into four integrals and consider

$$\begin{aligned}
\psi(w) &= \int_0^{\frac{1-w}{2}} \mathcal{K}(w+\Delta, \Delta)\,\mathrm{d}\Delta + \int_{\frac{1-w}{2}}^{1-w} \mathcal{K}(w+\Delta, \Delta)\,\mathrm{d}\Delta \\
&+ \int_{1-w}^{1-\frac{w}{2}} \mathcal{K}(w+\Delta-1, \Delta)\,\mathrm{d}\Delta + \int_{1-\frac{w}{2}}^1 \mathcal{K}(w+\Delta-1, \Delta)\,\mathrm{d}\Delta \\
&:= \psi_1(w) + \psi_2(w) + \psi_3(w) + \psi_4(w),
\end{aligned}$$

where $\psi_1, \psi_2, \psi_3, \psi_4$ denote each of the four integrals above. In order to analyse ψ_1, we use the change of variable $\Phi^{-1}(\Delta) = t$ (see also (6.2)) and obtain

$$\psi_1(w) = \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w+\Phi(t)), t)\rho(t)\,\mathrm{d}t.$$

For ψ_2, we use the change of variable $-\Phi^{-1}(w+\Delta) = t$, which in combination with (6.4) and the symmetry of K yields

$$\begin{aligned}
\psi_2(w) &= \int_{\Phi^{-1}(\frac{1-w}{2})}^{-\infty} K(-t, \Phi^{-1}(1-\Phi(t)-w))(-\rho(t))\,\mathrm{d}t \\
&= \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(-t, -\Phi^{-1}(w+\Phi(t)))\rho(t)\,\mathrm{d}t \\
&= \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w+\Phi(t)), t)\rho(t)\,\mathrm{d}t = \psi_1(w).
\end{aligned}$$

Turning now to ψ_3, we see that the change of variable $\Phi^{-1}(w+\Delta-1)=t$ yields

$$\psi_3(w)=\int_{-\infty}^{\Phi^{-1}(\frac{w}{2})} K(t,\Phi^{-1}(\Phi(t)-w+1))\rho(t)\,\mathrm{d}t.$$

It is easy to see that $\psi_3(w)=\psi_1(1-w)$ (using also the symmetry of K). Finally, for ψ_4, we use the change of variable $-\Phi^{-1}(\Delta)=t$ which together with (6.3) and (6.4) leads to

$$\begin{aligned}
\psi_4(w) &= \int_{\Phi^{-1}(\frac{w}{2})}^{-\infty} K(\Phi^{-1}(w+\Phi(-t)-1),-t)\rho(t)(-\,\mathrm{d}t)\\
&= \int_{-\infty}^{\Phi^{-1}(\frac{w}{2})} K(\Phi^{-1}(w+\Phi(-t)-1),-t)\rho(t)\,\mathrm{d}t\\
&= \int_{-\infty}^{\Phi^{-1}(\frac{w}{2})} K(\Phi^{-1}(w-\Phi(t)),-t)\rho(t)\,\mathrm{d}t\\
&= \int_{-\infty}^{\Phi^{-1}(\frac{w}{2})} K(-\Phi^{-1}(1-w+\Phi(t)),-t)\rho(t)\,\mathrm{d}t\\
&= \int_{-\infty}^{\Phi^{-1}(\frac{w}{2})} K(\Phi^{-1}(1-w+\Phi(t)),t)\rho(t)\,\mathrm{d}t=\psi_3(w),
\end{aligned}$$

where in the last step we once more used the symmetry of K. All these calculations show that we can write

$$\psi(w)=2\psi_1(w)+2\psi_1(1-w),\quad \forall w\in(0,1),$$

which proves the lemma. Let's also remark that $\psi(w)=\psi(1-w)$ for any $w\in(0,1)$, which indicates that ψ is symmetric alongside $w=1/2$. □

Next, we give a proof that the function ψ is convex for a specific kernel and density.

Lemma B.1 *If the kernel is given by* $K(x,y)=\pi e^{-2\pi|x-y|}$ *and* $\rho(x)=\frac{1}{2\lambda}e^{-|x|/\lambda}$ *with* $\lambda>0$*, then the function* ψ *(see also Lemma 6.5) is convex on* $(0,1)$.

Proof. Using the change of variable $\Phi^{-1}(\Delta)=t$, the expression of the ψ_1 becomes

$$\begin{aligned}
\psi_1(w) &= \int_{-\infty}^{\Phi^{-1}(\frac{1-w}{2})} K(\Phi^{-1}(w+\Phi(t))-t,0)\rho(t)\,\mathrm{d}t\\
&= \pi\int_0^{\frac{1-w}{2}} e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}\,\mathrm{d}\Delta,
\end{aligned}$$

where we also used that Φ^{-1} is increasing (see Section 6.1), so $\Phi^{-1}(w+\Delta) - \Phi^{-1}(\Delta) \geq 0$. Leibniz's rule in combination with (6.4) leads to:

$$\begin{aligned}\psi_1'(w) &= -\frac{\pi}{2}e^{-2\pi\left((\Phi^{-1}(\frac{1+w}{2})-\Phi^{-1}(\frac{1-w}{2})\right)} - 2\pi^2\int_0^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}}{\rho(\Phi^{-1}(w+\Delta))}\,\mathrm{d}\Delta \\ &= -\frac{\pi}{2}e^{4\pi\Phi^{-1}(\frac{1-w}{2})} - 2\pi^2\int_0^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}}{\rho(\Phi^{-1}(w+\Delta))}\,\mathrm{d}\Delta.\end{aligned}$$

Now by applying again Leibniz's rule, we obtain the second derivative of ψ_1 given by

$$\begin{aligned}\psi_1''(w) &= \frac{2\pi^2 e^{4\pi\Phi^{-1}(\frac{1-w}{2})}}{\rho(\Phi^{-1}(\frac{1-w}{2}))} \\ &\quad +2\pi^2\int_0^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}}{\rho^2(\Phi^{-1}(w+\Delta))}\left(2\pi + \frac{\rho'(\Phi^{-1}(w+\Delta))}{\rho(\Phi^{-1}(w+\Delta))}\right)\mathrm{d}\Delta.\end{aligned}$$

For the two-tailed exponential distribution $\rho(x) = \frac{1}{2\lambda}e^{-|x|/\lambda}$, it is easy to check that for $x \neq 0$, we can write

$$\frac{\rho'(x)}{\rho(x)} = -\frac{|x|}{\lambda x}.$$

From (6.3), it follows that $\Phi^{-1}(1/2) = 0$. Since $(1-w)/2 \leq 1/2$ and Φ^{-1} is increasing, it will follow that $\Phi^{-1}(\frac{1-w}{2}) \leq 0$. By making use of these results in the expression of $\psi_1''(w)$, we obtain:

$$\begin{aligned}\psi_1''(w) &= 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} \\ &\quad +2\pi^2\int_0^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}}{\rho^2(\Phi^{-1}(w+\Delta))}\left(2\pi - \frac{|\Phi^{-1}(w+\Delta)|}{\lambda\Phi^{-1}(w+\Delta)}\right)\mathrm{d}\Delta.\end{aligned}$$

We can split the integral in the expression of ψ_1'' into two parts to obtain

$$\begin{aligned}\psi_1''(w) &= 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} + 2\pi^2\int_0^{\frac{1}{2}-w} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}\left(2\pi+\frac{1}{\lambda}\right)}{\rho^2(\Phi^{-1}(w+\Delta))}\,\mathrm{d}\Delta \\ &\quad +2\pi^2\int_{\frac{1}{2}-w}^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}\left(2\pi-\frac{1}{\lambda}\right)}{\rho^2(\Phi^{-1}(w+\Delta))}\,\mathrm{d}\Delta.\end{aligned}$$

The first integral in the above is positive since the integrand always takes positive values. We can now write

$$\begin{aligned}\psi_1''(w) &\geq 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} + 2\pi^2\int_{\frac{1}{2}-w}^{\frac{1-w}{2}} \frac{e^{-2\pi(\Phi^{-1}(w+\Delta)-\Phi^{-1}(\Delta))}\left(2\pi-\frac{1}{\lambda}\right)}{\rho^2(\Phi^{-1}(w+\Delta))}\,\mathrm{d}\Delta \\ &= 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} - 2\pi^2\int_{\frac{1}{2}-w}^{\frac{1-w}{2}} e^{2\pi\Phi^{-1}(\Delta)}g'(\Delta)\,\mathrm{d}\Delta,\end{aligned}$$

where

$$g(\Delta) = 2\lambda e^{(\frac{1}{\lambda}-2\pi)\Phi^{-1}(w+\Delta)}.$$

This leads to

$$\begin{aligned}
\psi_1''(w) &\geq 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} - 2\pi^2 e^{2\pi\Phi^{-1}(\frac{1-w}{2})} \int_{\frac{1}{2}-w}^{\frac{1-w}{2}} g'(\Delta)\,\mathrm{d}\Delta \\
&= 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} - 2\pi^2 e^{2\pi\Phi^{-1}(\frac{1-w}{2})} \left(g\left(\frac{1-w}{2}\right) - g\left(\frac{1}{2}-w\right)\right) \\
&= 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} - 4\pi^2\lambda e^{(4\pi-\frac{1}{\lambda})\Phi^{-1}(\frac{1-w}{2})} + 4\pi^2\lambda e^{2\pi\Phi^{-1}(\frac{1-w}{2})} \\
&= 4\pi^2\lambda e^{2\pi\Phi^{-1}(\frac{1-w}{2})} \geq 0, \quad \forall w \in (0,1).
\end{aligned}$$

□

Finally, let us remark that following the same idea, we can prove a similar result for Gaussian distributions, which occur frequently in practical applications. So, it makes sense to assume that the result given by Lemma B.1 has some generality.

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