# Randomized Algorithms for High-Dimensional Integration and Approximation

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# Chapter 1

# Introduction

Let $F$ be a separable Hilbert space of functions defined on some non-empty domain $D$, and $G$ be a separable Hilbert space. We are considering a linear bounded operator $S : F \to G$, $S$ may be for example the integration functional or the embedding operator. The linear approximation problem is to approximate $S$ with the help of simpler operators. In many applications coming from biology, medicine, engineering and other fields $D \subset \mathbb{R}^d$ for large $d$. In that case one talks of high-dimensional approximation, which is the focus of this dissertation.

In this Introduction we present one of the most prominent approximation problems: high-dimensional integration.

## 1.1 Problem Formulation

High-dimensional integration belongs to the most pronounced problems of numerical analysis. With applications ranging from financial mathematics to physics and chemistry, it is important for practitioners and attracts interest from the theoretical point of view. Generally, a non-empty domain $D \subset \mathbb{R}^d$ is given (where $d$ is thought of as 'large', what this concretely means depends on the problem at hand) and one is asked to devise an algorithm which approximates $S(f) = \int_D f(x)\,\mu(dx)$ well for all $f$ from some normed space of functions $F$ and some finite measure $\mu$ on $D$. The space $F$ is usually called input space.

Two things need to be cleared at this point. Firstly, an *algorithm* is, loosely speaking, a mapping of the form $\phi \circ N$, where $N : F \to \mathbb{R}^n$ is an *information operator* given by $N(f) = (L_1(f), \ldots, L_n(f))$ for some (linear) functionals $L_1, \ldots, L_n \in F'$, and $\phi : \mathbb{R}^n \to \mathbb{R}$ is any mapping. Here $n$ may be fixed or random or even dependent on the input $f$. Also the functionals used may be deterministic or random. For a precise mathematical definition of algorithms we refer to Chapter 3. Here we only note that a mapping $A$ is called a *randomized algorithm* if it maps from some probability space into the class of deterministic algorithms, and for every $f$ from the input space $Af$ is a random variable.

Secondly, one must say what does good approximation mean. The typical error criterion used in the case of deterministic algorithms is the *deterministic worst case error*

given by

$$e^{\mathrm{d}}(S,A) = \sup_{f\in F, \|f\|_F\leq 1} |(S-A)f|, \tag{1.1}$$

where $S$ denotes the integration operator and $A$ is the algorithm. (The input space is already implicitly contained in the problem formulation.) The deterministic worst case error allows for different generalizations when considering randomized algorithms. The ones which are of the most interest to us are the *randomized worst case error*

$$e^{\mathrm{w}}(S,A) = \left(\mathbf{E}\left[\sup_{f\in F, \|f\|_F\leq 1} |(S-A)f|\right]^2\right)^{\frac{1}{2}}, \tag{1.2}$$

and the *randomized mean square error*, often referred to just as randomized error

$$e^{\mathrm{r}}(S,A) = \left(\sup_{f\in F, \|f\|_F\leq 1} \mathbf{E}\left[|(S-A)f|\right]^2\right)^{\frac{1}{2}}. \tag{1.3}$$

## 1.2 Challenges in the High Dimension

A linear algorithm for numerical integration meant to approximate $\int_D f(x)\mu(dx)$ is of the form

$$Af = \sum_{j=1}^{N} w_j f(x_j),$$

with some scalar *weights* $w_j$ and *sampling points* $x_j \in D, (j = 1, \ldots, N)$, (the number of evaluations $N$, weights and sampling points may be fixed or random variables, they may also depend on the concrete input). Such algorithms are often called *quadratures*. Devising an algorithm usually boils down to finding good weights and sampling points, a thing that even in one dimension may be quite tricky. Needles to say that increasing the dimension makes the problem even more demanding.

In one dimension one usually seeks for quadratures which are exact on polynomials of possibly high degree. Since devising a quadrature based on $N$ integration nodes one has at his disposal $2N$ decision variables ($N$ nodes and $N$ weights) it comes as no surprise that one is able to come up with a quadrature (the so-called Gauss quadrature) which is exact on all polynomials of degree smaller or equal $2N-1$. Still, this requires solving a system of $2N$ non-linear equations. One could try to use the same idea in more dimensions. Suppose we want to integrate exactly all the monomials in $d$ variables of degree smaller or equal $n$. The dimension of the space spanned by them is $\binom{d+n}{d}$, so to define the algorithm we need to solve a system of $\binom{d+n}{d}$ non-linear equations. Moreover, to ascertain that such quadrature exists we usually need to allow for $N \geq \frac{1}{2}\binom{d+n}{d}$ integration nodes. Even for moderate dimension $d$ it becomes impracticable.

Another idea would be to use product rules. Suppose for instance that $D = [0,1)^d$, and we have good quadratures $A_1, \ldots, A_d$, for integrating functions on $[0,1)$. Denote

by $(p_j^{(i)})_{j=1}^n$ the sampling points used by $A_i$. One could try to devise an algorithm for integration on $D$ by taking the tensor product grid, i.e. the grid consisting of all the points of the form $(p_{j_1}^{(1)}, \ldots, p_{j_d}^{(d)}), j_1, \ldots, j_d = 1, \ldots, n$, but then one would end up with an algorithm sampling at $n^d$ points, which even for moderate $n$ and $d$ is prohibitive. If one now considers (as one would like to do in practice) a compound quadrature, i.e. divides $[0,1)^d$ into $k^d$ cubes of equal volume (where $k$ is much bigger then $n$) and uses rescaled version of the product rule quadrature on each of those subcubes one obtains (in appropriate function spaces) an integration error of the order $k^{-n}$. For that one uses $N = (kn)^d$ sampling points, i.e. the error in terms of the number of sampling points used is of the order $N^{-\frac{n}{d}}$, which is unsatisfactory for large $d$.

For sure, algorithms using 'sparser' sampling points are needed. Finding such 'sparse' sampling points which nevertheless yield good approximation of the integral is generally seen as a challenging problem.

One speaks of the *curse of dimensionality*, meaning different phenomena arising when dealing with high-dimensional problems which make them much more difficult to solve then the lower-dimensional problems. Informally speaking we have seen two emanations of the curse discussing multidimensional Gauss rules and product rules. The phrase, coined by R. Bellman when considering dynamic programming, may be made precise in more than one way, depending on the branch of mathematics at hand. Probably the most suitable one when talking about high-dimensional numerical integration is the one that is stated using the language of information-based complexity, saying basically that the complexity of an integration problems often increases exponentially with the dimension. This is true above all in the worst case setting. For more information on this subject we refer to three volumes [84, 85, 86] of the monograph on information-based complexity.

## 1.3 Overview of Algorithms Used for High-Dimensional Integration

When describing typical algorithms we shall confine ourselves to integration with respect to the Lebesgue measure on $\mathbb{R}^d$, denoted by $\lambda^d$, and consider $D$ with $0 < \lambda^d(D) < \infty$ - this enables us to assume without loss of generality that $\lambda^d(D) = 1$.

The algorithms usually applied to the problem of high-dimensional integration fall into a few categories:

1. Monte Carlo methods,
2. (deterministic/randomized) quasi-Monte Carlo methods,
3. the Smolyak method,
4. mixed algorithms.

Before we start an overview of those methods it is worthwhile to think for a moment about the advantages and disadvantages of randomized algorithms as compared to the

deterministic ones. The biggest disadvantage is that randomized algorithms usually do not give a guarantee of providing a good approximation. Still, they may guarantee good approximation with arbitrarily high probability. Usually, the convergence rate of randomized algorithms (when taking into account the randomized root mean square error) is higher then the convergence rate of the 'corresponding' deterministic algorithms. What is however most important, randomized algorithms enable us to repeat the experiments and use then the whole machinery of Statistics to obtain a good approximation of the integral.

The most widely used randomized methods are without doubt *(plain or simple) Monte Carlo (MC) quadratures.* Let $f \in L^2(D)$ and suppose that we have a supply of $N$ independent random variables $(X_j)_{j=1}^N$ distributed uniformly on $D$. The (plain or simple) Monte Carlo quadrature $Q_N^{\mathrm{MC}}$ is then given by

$$Q_N^{\mathrm{MC}} f = \frac{1}{N} \sum_{j=1}^{N} f(X_j). \tag{1.4}$$

Due to the independence of $(X_j)_{j=1}^N$ we have

$$\mathbf{E}\left[(S - Q_N^{\mathrm{MC}})f\right]^2 = \frac{\mathrm{Var}(f)}{N}, \tag{1.5}$$

which gives an error of the order $\mathcal{O}(N^{-\frac{1}{2}})$. Even though the convergence rate may seem to be far from impressive, the big advantage of the Monte Carlo quadrature is that its convergence rate is independent of the dimension. Note that the assumptions on $f$ are very mild, it suffices that it is square-integrable. More problematic are the assumptions on $D$. To use the Monte Carlo quadrature in practice one needs to be able to sample from the uniform distribution on $D$, which in many cases may be difficult.

When applying plain Monte Carlo there is no hope of beating the square-root convergence. A lot of effort though has been put into reducing the constant, resulting in many *variance reduction methods*, which are of big practical interest. To name just the most prominent ones: antithetic sampling (i.e., loosely speaking, using pairwise negatively correlated random variables instead of the independent ones), importance sampling (changing the underlying measure to obtain more samples in the area where the integrand is more variable), stratified sampling (dividing $D$ into $N$ areas of volume $N^{-1}$ and sampling just one point from every of those areas) and control variate (substracting from $f$ a function $g$ which is at the same time close to $f$ in some sense and simple to integrate, and applying plain Monte Carlo to $f - g$).

The question that arises is: knowing more about the underlying input space, can we do better? The answer is in many cases 'yes'. Further on we shall assume that $D = [0,1)^d$. The intuition is that more 'regular' sampling points should give better integration nodes then just points chosen uniformly at random. That is how the *quasi-Monte Carlo (QMC)* integration started. A quasi-Monte Carlo quadrature $Q_N^{\mathrm{QMC}}$ is just a quadrature of the form

$$Q_N^{\mathrm{QMC}} f = \frac{1}{N} \sum_{j=1}^{N} f(p_j), \tag{1.6}$$

where $P = (p_j)_{j=1}^N$ is some (deterministic) point set in $[0,1)^d$. The big limitation of QMC is that we usually have to assume a lot of regularity on $D$ (as in our case, $D = [0,1)^d$). Also, if one allows for any input $f \in L^2([0,1)^d)$, then there is no big hope of having a better convergence rate then in the Monte Carlo setting. However, there are still 'large' input spaces for which concrete quasi-Monte Carlo methods perform very well.

Here we give a short example. We take the $d$-dimensional Korobov space with smoothness parameter $r > \frac{1}{2}$ as input space. The $d$-dimensional Korobov space $K_r([0,1)^d)$ is just the $d$-fold tensor product of one-dimensional Korobov spaces with smoothness $r > \frac{1}{2}$, $K_r([0,1))$, which in turn are given by

$$K_r([0,1)) := \{f \in L^2([0,1)) : |\hat{f}(0)| + \sum_{k \in \mathbb{Z}\setminus\{0\}} |\hat{f}(k)|^2 |k|^{2r} < \infty\},$$

where $\hat{f}(k) = \int_{[0,1)} f(x) e^{-2\pi k x}\, dx$ is the $k$-th Fourier coefficient of $f$. We consider a quasi-Monte Carlo quadrature based on a rank-1 lattice. Let $N$ be prime. A rank-1 lattice consists of points of the form

$$kg \mod 1, \quad \mathrm{k} = 0, 1, \ldots, \mathrm{N}-1,$$

where the so-called generating vector $g$ is an element of $\{1, \ldots, N-1\}^d$. For a more detailed discussion we refer to Chapter 5. It may be shown that there exists a generating vector (more precisely, a sequence of generating vectors) such that the deterministic worst-case error satisfies in this setting $\mathcal{O}_{r,d}(\frac{\log(N)^{rd}}{N^r})$. This has been originaly proven by E. Hlawka. For a nice exposition see [74, Chapter 4].

Another prominent class of good quasi-Monte Carlo points is the class of $(0,m,d)$-*nets*, introduced by H. Niederreiter in [78]. To describe them we first need to define elementary intervals. Given $b \in \mathbb{N}_{\geq 2}$, an interval of the form $[\frac{k}{b^l}, \frac{k+1}{b^l}), l \in \mathbb{N}, k \in \{0, 1, \ldots, b^l - 1\}$ is called elementary in base $b$. Now an elementary interval in $d$ dimensions is just a Cartesian product of one-dimensional elementary intervals in the same base. A point set $P$ is a $(0,m,d)$-net in base $b$ if every $d$-dimensional elementary interval $E$ in base $b$ with $\lambda^d(E) = b^{-m}$ contains exactly one point from $P$. There are explicit constructions yielding efficiently $(0,m,d)$-nets at least in moderate dimensions (the so-called *digital nets*).

To get the best of both worlds of MC and QMC quadratures one uses *randomized quasi-Monte Carlo (RQMC)* methods. The basic idea is to start with a 'good' QMC point set and then randomize it, so as to preserve some special structure or regularity. An example would be shifted rank-1 lattices. Let $P = (p_j)_{j=1}^N$ be a rank-1 lattice in $[0,1)^d$. We define a (random) point set $\tilde{P}$ via $\tilde{P} = (\tilde{p}_j)_{j=1}^N$ where $\tilde{p}_j = p_j + U \mod 1, \mathrm{j} = 1, \ldots, \mathrm{N}$, with a random variable $U$ uniformly distributed on $[0,1)^d$.

The typical way of randomizing a $(0,m,d)$-net is via scrambling. A bijective mapping $\sigma : [0,1)^d \to [0,1)^d$ is called a scrambling of depth $m$ (in base $b$) if for every elementary interval $E$ in base $b$ with $\lambda^d(E) \geq b^{-m}$ it holds that $\sigma(E)$ is an elementary interval and $\lambda^d(E) = \lambda^d(\sigma(E))$. Random scrambling $\sigma$ (of depth $m$) may be easily constructed in such a way that for every $x \in [0,1)^d$ the random variable $\sigma(x)$ is uniformly distributed in $[0,1)^d$. Given a $(0,m,d)$-net $P$ and a random scrambling $\sigma$ the (random) point set $\tilde{P} = \sigma(P)$ is

called scrambled $(0, m, d)$-net. Note that, in particular, a scrambled $(0, m, d)$-net is almost surely a $(0, m, d)$-net. The concept of scrambling has been introduced and investigated by A.B. Owen, see [90].

Quite often, even if theoretical constructions of 'good' QMC points are known, generating them in high dimension $d$ may be expensive or simply difficult. In those situations it pays off to use lower-dimensional point sets and to combine them to create a high dimensional point set. One of the most successful methods of combining lower dimensional quadratures is via the so-called Smolyak algorithm. Suppose e.g. we have $d$ sequences $(U_l^{(n)})_{l\in\mathbb{N}}, n = 1, \dots, d$, of $s$-dimensional QMC quadratures, where for a fixed $n$ the number of points used by a quadrature grows with $l$. We extend the definition by putting $U_0^{(n)} = 0, n = 1, \dots, d$, and consider the differences $\Delta_l^{(n)} = U_l^{(n)} - U_{l-1}^{(n)}$. We define the $d$-dimensional Smolyak algorithm of level $L \geq d$ by

$$A(L, d) = \sum_{\mathbf{l}\in Q(L,d)} \bigotimes_{n=1}^{d} \Delta_{l_n}^{(n)}, \tag{1.7}$$

where $Q(L, d) := \left\{\mathbf{l} \in \mathbb{N}^d \mid \|\mathbf{l}\|_1 \leq L\right\}$. Now, $A(L, d)$ is a quadrature in $sd$ dimensions. A rule of the thumb is that if for every $n = 1, \dots, d$, the rate of convergence of $(U_l^{(n)})_{l\in\mathbb{N}}$ is $\mathcal{O}(N^{-\alpha})$ then the convergence rate of Smolyak algorithm $(A(L, d))_{L\geq d}$ is $\mathcal{O}(\frac{\log(N)^{(d-1)(\alpha+1)}}{N^{\alpha}})$, i.e. the Smolyak algorithm performs really well for moderate $d$. In higher dimension the Smolyak algorithm is interesting as a building block of more complicated algorithms. Note that in general, even if all the algorithms $U_l^{(n)}$ are QMC quadratures, the associated Smolyak method needs not be a QMC quadrature. The Smolyak method has been introduced in [104], a revival of interest in it is marked by the article [116]. For details and an application to infinite-dimensional integration we refer to Chapters 3 and 4.

In many high-dimensional integration problems some coordinates are more 'important' then the others, i.e. for example the function we want to integrate is more variable in some directions. It stands to reason to use more expensive but at the same time more precise integration methods on those coordinates and combine them with some cheaper methods (usually Monte Carlo) on the other coordinates. This gives rise to the mixed methods.

An important question would be now: how to asses the goodness of a given QMC point set? A possible answer is given by the discrepancy. The local discrepancy at $x \in [0, 1)^d$ of a point set $P$ consisting of $N$ points is given by

$$D(P, x) := \left| \frac{|P \cap [0, x)|}{N} - \lambda^d([0, x)) \right|.$$

The value of interest, the so-called star discrepancy $D^*(P)$, is

$$D^*(P) = \|D(P, \cdot)\|_\infty.$$

It turns out that for functions with bounded Hardy-Krause variation the error made by integrating the function with the help of a QMC quadrature based on a point set $P$ is

bounded from above by the product of the Hardy-Krause variation (depending only on the function at hand) and the star discrepancy of $P$. For more information on discrepancy, see Section 2.3.

## 1.4 Our Contribution

In Chapter 3 we start a thorough investigation of the randomized Smolyak method, i.e. the Smolyak method with building blocks being randomized algorithms (or more generally, randomized operators). This is a general construction made to deal with high-dimensional approximation problems and its applicability is not restricted to high-dimensional integration. The important feature of the randomization considered is that the sequences of building blocks $(U_l^{(n)})_{l\in\mathbb{N}}, n = 1, \dots, d$, are assumed to be independent.

In the first part of the chapter we give a detailed error analysis based on [116], where analogous results were obtained for the deterministic case. We focus on the randomized worst case error and the randomized root mean square error. The basic idea is to show how the convergence rate of building blocks transfers to the convergence rate of the Smolyak algorithm. In particular, we show that if the building blocks exhibit convergence rate $\Theta(N^{-\alpha})$ for some $\alpha > 0$, then under some mild additional assumptions the convergence rate of the Smolyak method satisfies for any $\epsilon > 0$ and $\mathrm{x} \in \{\mathrm{w}, \mathrm{r}\}$

$$e^{\mathrm{x}}(S, A(L, d)) = \mathcal{O}\left(\frac{\log(N)^{(\alpha+1)(d-1)}}{N^{\alpha}}\right), \tag{1.8}$$

and

$$e^{\mathrm{x}}(S, A(L, d)) = \Omega\left(\frac{\log(N)^{\alpha(d-1-\epsilon)}}{N^{\alpha}}\right). \tag{1.9}$$

Moreover, in the upper bounds, we are able to determine the dependence of implicit constants on $d$.

In the second part of the chapter we combine our results on the convergence rate of the Smolyak algorithm with the results from [97] on multivariate decomposition methods and embedding results from [42] to prove a sharp result on the polynomial order of convergence of the $N$-th minimal error for randomized infinite-dimensional integration in the case of general weighted reproducing kernel Hilbert spaces. The statement is basically that if the weights decay fast enough, the infinite-dimensional integration problem is (essentially) no harder then the corresponding one-dimensional integration problem.

In Chapter 4 we exploit the fact that in the general setting from Chapter 3 there is a gap between the upper bound (1.8) and the lower bound (1.9) on the convergence of the Smolyak method. Inspired by [55] we consider a concrete example of integrating $ds$-variate functions from Haar-wavelet spaces with smoothness parameter $\alpha > \frac{1}{2}$ with the help of the Smolyak method, where for every $n = 1, \dots, d$, and $l \in \mathbb{N}$ the building block $U_l^{(n)}$ is an RQMC quadrature based on a scrambled $(0, l-1, s)$-net. Moreover, we assume that all the $U_l^{(n)}, n = 1, \dots, d, l \in \mathbb{N}$, are randomized independently. As an error criterion we consider the randomized root mean square error. It is known (see [55])

that the convergence rate of RQMC quadratures based on scrambled nets in Haar-wavelet space with smoothness $\alpha > \frac{1}{2}$ is of the order $\Theta(N^{-\alpha-\frac{1}{2}})$. We show that one obtains a convergence rate of the Smolyak algorithm

$$e^{\mathrm{r}}(S, A(L,d)) = \Theta\left(\frac{\log(N)^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}\right)$$

as opposed to $\mathcal{O}(\frac{\log(N)^{(d-1)(\alpha+\frac{3}{2})}}{N^{\alpha+\frac{1}{2}}})$ and $\Omega(\frac{\log(N)^{(\alpha+\frac{1}{2})(d-1-\epsilon)}}{N^{\alpha+\frac{1}{2}}})$ which may be deduced from Chapter 3 (note that the parameter $\alpha$ has in both chapters a different meaning).

Chapter 5 deals with different notions of negative dependence of sampling schemes: pairwise negative dependence and negative dependence. A finite randomized point set $\mathcal{P} = (p_j)_{j=1}^N$ in $[0,1)^d$ is called a sampling scheme if every $p \in \mathcal{P}$ is distributed uniformly in $[0,1)^d$ and the distribution of $(p_{\pi(j)})_{j=1}^N$ is the same as the distribution of $(p_j)_{j=1}^N$ for any permutation $\pi$ of $\{1,2,\ldots,N\}$. Using pairwise negatively dependent sampling schemes as integration nodes may be seen as a variance reduction technique closely related to antithetic sampling. On the other hand, negatively dependent sampling schemes exhibit with high probability low discrepancy.

Chapter 5 is on the one hand thought of as an overview on negative dependence of sampling schemes, but on the other hand it contains also new results. In particular we give new examples of negatively dependent sampling schemes, namely generalized stratified sampling and randomly shifted and jittered rank-1 lattices. We argue that resigning from any step of the proposed randomization of rank-1 lattices infringes either the sampling scheme property or the pairwise negative dependence. Moreover, we compare our construction with the Latin hypercube sampling which is known to be negatively dependent, see [41]. We show that concatenating two negatively dependent sampling schemes results in a negatively dependent sampling scheme. Finally, we compare the notions of negative dependence and pairwise negative dependence, showing that there are negatively dependent sampling schemes which are not pairwise negatively dependent and vice versa. We also supply a theorem on discrepancy bounds for negatively dependent sampling schemes, similar in taste to Theorem 4.3. from [41].

Chapters 3 an 4 are slightly modified versions of research articles, respectively, [46] and [121]. Chapter 5 combines the articles [120] and [122].

# Chapter 2

# Preliminaries

## 2.1 Tensor Product of Hilbert Spaces

The presentations basically follows [119].

In order to define the tensor product of Hilbert spaces we first need the notion of the algebraic tensor product of vector spaces. Let $X$ and $Y$ be two vector spaces over (the same) field $\mathbb{K}$. We denote by

$$F(X,Y) := \left\{ \sum_{j=1}^{m} c_j(x_j, y_j) \,|\, c_j \in \mathbb{K}, m \in \mathbb{N}, x_j \in X, y_j \in Y \right\},$$

the formal linear combinations of pairs $(x, y) \in X \times Y$. Let $N = N(X,Y)$ be the subspace of $F(X,Y)$ consisting of all the elements of the form

$$\sum_{j=1}^{m}\sum_{k=1}^{n} a_j b_k (x_j, y_k) - \left( \sum_{j=1}^{m} a_j x_j, \sum_{k=1}^{n} b_k y_k \right), \quad a_j, b_k \in \mathbb{K}, x_j \in X, y_k \in Y.$$

We define a new vector space called *(algebraic) tensor product of $X$ and $Y$* and denoted by $X \widetilde{\otimes} Y$ via

$$X \widetilde{\otimes} Y := F(X,Y)/N(X,Y).$$

The equivalence class generated by a pair $(x, y)$ is denoted by $x \otimes y$.

Let now $(H_1, \langle\cdot,\cdot\rangle_1)$ and $(H_2, \langle\cdot,\cdot\rangle_2)$ be Hilbert spaces. We define on $H_1 \widetilde{\otimes} H_2$ a sesquilinear form

$$s\left( \sum_{j=1}^{m} c_j x_j \otimes y_j, \sum_{k=1}^{n} c'_k x'_k \otimes y'_k \right) := \sum_{j=1}^{m}\sum_{k=1}^{n} \bar{c}_j c'_k \langle x_j, x'_k\rangle_1 \langle y_j, y'_k\rangle_2, \quad c_j, c'_k \in \mathbb{K}, x_j, x'_k \in H_1, y_j, y'_k \in H_2.$$

One easily sees that $s$ is actually an inner product on $H_1 \widetilde{\otimes} H_2$, which we denote by $\langle\cdot,\cdot\rangle$. The completion of $(H_1 \widetilde{\otimes} H_2, \langle\cdot,\cdot\rangle)$ with respect to $\langle\cdot,\cdot\rangle$ is called the *tensor product of (Hilbert spaces) $H_1$ and $H_2$*. We denote this completion by $H_1 \otimes H_2$. Elements of the form $h_1 \otimes h_2, h_1 \in H_1, h_2 \in H_2$ are called *elementary tensors*.

Let $K_1, K_2$ be two further Hilbert spaces. For bounded linear operators $T_1 : H_1 \to K_1$ and $T_2 : H_2 \to K_2$ we define the *tensor product operator* $T_1 \otimes T_2 : H_1 \otimes H_2 \to K_1 \otimes K_2$ by setting

$$(T_1 \otimes T_2)(h_1 \otimes h_2) := (T_1 h_1) \otimes (T_2 h_2)$$

for every elementary tensor $h_1 \otimes h_2 \in H_1 \otimes H_2$.

**Lemma 2.1.1.** *Let $T_1$ and $T_2$ be as above. The tensor product operator $T_1 \otimes T_2$ is then bounded and it holds $\|T_1 \otimes T_2\|_{\mathrm{op}} = \|T_1\|_{\mathrm{op}} \|T_2\|_{\mathrm{op}}$.*

**Example 2.1.2.** *Let $(\Omega_1, \Sigma_1, \mu_1)$ and $(\Omega_2, \Sigma_2, \mu_2)$ be measure spaces with $\sigma$-finite measures $\mu_1, \mu_2$. Abusing the notation we write $\mu_1 \otimes \mu_2$ for the product measure of $\mu_1$ and $\mu_2$. We are considering a linear operator*

$$\Gamma : F(L^2(\Omega_1, \mu_1), L^2(\Omega_2, \mu_2)) \to L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$$

*which sends an element $\sum_{j=1}^n c_j (f_j, g_j)$ to a function $(x, y) \mapsto \sum_{j=1}^n c_j f_j(x) g_j(y)$. It may be easily seen that $\ker(\Gamma) = N(L^2(\Omega_1, \mu_1), L^2(\Omega_2, \mu_2))$, so the first homomorphism theorem guarantees that the mapping*

$$\widetilde{\Gamma} : L^2(\Omega_1, \mu_1) \widetilde{\otimes} L^2(\Omega_2, \mu_2) \to L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$$

*which sends $\sum_{j=1}^n c_j f_j \otimes g_j$ to a function $(x, y) \mapsto \sum_{j=1}^n c_j f_j(x) g_j(y)$ is injective. Moreover, $\widetilde{\Gamma}$ is isometric. Indeed, denoting by $\langle \cdot, \cdot \rangle_1, \langle \cdot, \cdot \rangle_2, \langle \cdot, \cdot \rangle$ scalar products on $L^2(\Omega_1, \mu_1), L^2(\Omega_2, \mu_2)$ and $L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$, respectively, we obtain*

$$\langle \widetilde{\Gamma}(f \otimes g), \widetilde{\Gamma}(h \otimes k) \rangle^2 = \langle fg, hk \rangle^2 = \int_{\Omega_1 \times \Omega_2} f(x) g(y) h(x) k(y) (\mu_1 \otimes \mu_2)(dx, dy)$$

$$= \int_{\Omega_1} f(x) h(x) \mu_1(dx) \int_{\Omega_2} g(y) k(y) \mu_2(dy) = \langle f, h \rangle_1^2 \langle g, k \rangle_2^2 = \langle f \otimes g, h \otimes k \rangle^2_{L^2(\Omega_1, \mu_1) \otimes L^2(\Omega_2, \mu_2)}.$$

*As an isometric injection $\widetilde{\Gamma}$ may be extended to isometry $\overline{\Gamma}$ and the surjectivity of $\overline{\Gamma}$ follows since $\mu_1, \mu_2$ are $\sigma$-finite. As a result $L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$ as a Hilbert space is isometric isomorphic to $L^2(\Omega_1, \mu_1) \otimes L^2(\Omega_2, \mu_2)$.*

*If not stated otherwise for a Hilbert subspace $H_1 \otimes H_2$ of $L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$ we always identify $h_1 \otimes h_2 \in H_1 \otimes H_2$ with a function $h : \Omega_1 \times \Omega_2 \to \mathbb{K}, (x, y) \mapsto h_1(x) h_2(y)$.*

## 2.2 Reproducing Kernel Hilbert Spaces

The following presentation is based on [4, 17, 74]

Let $D \neq \emptyset$ be a set, $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, and $(H, \langle \cdot, \cdot \rangle)$ be any Hilbert space of $\mathbb{K}$-valued functions with domain $D$.

**Definition 2.2.1.** A function $K : D \times D \to \mathbb{C}$ satisfying

1. $K(\cdot, y) \in H$, for every $y \in D$,

2. $\langle f, K(\cdot, y)\rangle = f(y)$, for every $f \in H$ and $y \in D$,

is called a *reproducing kernel of H.* The second condition is known as the *reproducing property.*

Using the reproducing property one easily sees that if a reproducing kernel for $H$ exists, then it is unique. Hilbert spaces admitting a reproducing kernel are called *reproducing kernel Hilbert spaces (RKHS).*The next theorem answers an important question: when does a Hilbert space of functions admit a reproducing kernel? A special case may be found e.g. as [74, Thm 3.5.] and proof in the general case is virtually the same.

**Theorem 2.2.2.** *A Hilbert space of functions $H$ admits a reproducing kernel if and only if every evaluation functional on $H$ is continuous, i.e. for every $x \in D$ the functional $\xi_x : H \to \mathbb{K}$ given by $\xi_x(f) = f(x)$ is continuous.*

Theorem 2.2.2 explains at least partially why RKHS are so important in the theory of numerical integration.

It is not difficult to see (proofs may be found e.g. in [4]) that if $K$ is a reproducing kernel of $(H, \langle\cdot,\cdot\rangle)$ then it is hermitian (i.e. $K(x,y) = \overline{K(y,x)}$ for every $x, y \in D$) and positive semi-definite (i.e. for any choice of $m \in \mathbb{N}, x_1, \ldots, x_m \in D$ and $\xi_1, \ldots, \xi_m \in \mathbb{C}$ one has $\sum_{i,j=1}^{m} \bar{\xi}_i \xi_j K(x_i, x_j) \geq 0$).

The following Moore-Aronszajn theorem yields a converse to the above.

**Theorem 2.2.3.** *Let $D \neq \emptyset$. Suppose that $K : D \times D \to \mathbb{C}$ is a hermitian, positive semi-definite function. Then there exists uniquely determined Hillbert space $(H, \langle\cdot,\cdot\rangle)$ with reproducing kernel $K$.*

Because of the Moore-Aronszajn theorem we may talk just of reproducing kernels, without specifying explicitly the underlying Hilbert space.

**Example 2.2.4.** *1. From the Moore-Aronszajn theorem we know that for any $D \neq \emptyset$ the function $K : D \times D \to \mathbb{R}$ given by $K \equiv 1$ is a reproducing kernel for some Hilbert space $H$. Since for every $f \in H$ and $y, z \in D$ we have*

$$f(y) = \langle f, K(\cdot, y)\rangle = \langle f, K(\cdot, z)\rangle = f(z)$$

*we see that $H$ consists just of constant functions and for $f, g \in H$ with $f \equiv \alpha, g \equiv \beta$ it holds $\langle f, g\rangle = \alpha\beta$.*

*2. For $k \in \mathbb{Z}$ and $f \in L^2([0,1))$ we denote by $\hat{f}(k)$ the $k$-th Fourier coefficient of $f$, given by $\hat{f}(k) := \int_{[0,1)} f(x)e^{-2\pi ikx}dx$. Let $r > \frac{1}{2}$. The space of functions*

$$K_r([0,1)) := \{f \in L^2([0,1)) : |\hat{f}(0)| + \sum_{k\in\mathbb{Z}\setminus\{0\}} |\hat{f}(k)|^2|k|^{2r} < \infty\},$$

*equipped with the scalar product*

$$\langle f, g\rangle = \hat{f}(0)\hat{g}(0) + \sum_{k\in\mathbb{Z}\setminus\{0\}} \hat{f}(k)\overline{\hat{g}(k)}|k|^{2r}$$

*is called* Korobov space with smoothness $r$. *We show that the function*

$$K_r : [0,1)^2 \to \mathbb{C}, (x,y) \mapsto 1 + \sum_{l \in \mathbb{Z}\setminus\{0\}} \frac{e^{2\pi i l(x-y)}}{|l|^{2r}}$$

*is the reproducing kernel of* $K_r([0,1))$.

*First note that* $\widehat{K_r(\cdot,y)}(0) = 1$ *and for* $k \neq 0$ *we have*

$$\begin{aligned}\widehat{K_r(\cdot,y)}(k) &= \int_{[0,1)} \left(1 + \sum_{l \in \mathbb{Z}\setminus\{0\}} \frac{e^{2\pi i l(x-y)}}{|l|^{2r}}\right) e^{-2\pi i k x} dx \\ &= \int_{[0,1)} \frac{e^{-2\pi i k y}}{|k|^{2r}} dx = \frac{e^{-2\pi i k y}}{|k|^{2r}}.\end{aligned}$$

*Since* $r > \frac{1}{2}$ *it follows immediately that* $|\widehat{K_r(\cdot,y)}(0)| + \sum_{k \in \mathbb{Z}\setminus\{0\}} |\widehat{K_r(\cdot,y)}(k)|^2 |k|^{2r} < \infty$, *so* $K_r(\cdot,y) \in K_r([0,1))$. *Moreover,*

$$\begin{aligned}\langle f, K_r(\cdot,y)\rangle &= \hat{f}(0)\widehat{K_r(\cdot,y)}(0) + \sum_{l \in \mathbb{Z}\setminus\{0\}} \hat{f}(l)\overline{\widehat{K_{r(\cdot,y)}}(l)}|l|^{2r} \\ &= \hat{f}(0) + \sum_{l \in \mathbb{Z}\setminus\{0\}} \hat{f}(l) e^{-2\pi l y} = f(y),\end{aligned}$$

*so the reproducing property also holds.*

Let now $K_i : D \times D \to \mathbb{C}, i = 1,2$, be reproducing kernels. Due to the Moore-Aronszajn theorem it is clear that $K_1 + K_2$ and $K_1 \otimes K_2$ are also reproducing kernels. What is important, knowing Hilbert spaces $H_1$ and $H_2$ corresponding to $K_1$ and $K_2$ respectively, we may easily find Hilbert spaces corresponding to $K_1 + K_2$ and $K_1 \otimes K_2$. Theorems 2.2.5 and 2.2.6 come from [4].

**Theorem 2.2.5.** *If* $K_i, i = 1,2$, *are reproducing kernels of Hilbert spaces* $(H_i, \langle\cdot,\cdot\rangle_i)$ *then* $K := K_1 + K_2$ *is the reproducing kernel of the Hilbert space* $H$ *consisting of all the functions of the form* $f = f_1 + f_2, f_1 \in H_1, f_2 \in H_2$ *and equipped with the norm*

$$\|f\|^2 = \inf_{f_1 \in H_1, f_2 \in H_2 : f = f_1 + f_2} \left(\|f_1\|_1^2 + \|f_2\|_2^2\right),$$

*where* $\|\cdot\|_i$ *is the norm induced by* $\langle\cdot,\cdot\rangle_i$.

The statement is particularly simple if $H_1 \cap H_2 = \{0\}$, which implies that the decomposition $f = f_1 + f_2, f_1 \in H_1, f_2 \in H_2$, is unique.

**Theorem 2.2.6.** *Let* $H_1, H_2$ *be reproducing kernel Hilbert spaces with kernels* $K_1$ *and* $K_2$ *respectively. The tensor product space* $H := H_1 \otimes H_2$ *admits the reproducing kernel* $K = K_1 \otimes K_2$, *i.e. given for every* $x_1, x_2, y_1, y_2 \in D$ *by*

$$K((x_1,x_2),(y_1,y_2)) = K_1(x_1,y_1)K_2(x_2,y_2).$$

## 2.3 Discrepancy

Let $d \in \mathbb{N}$. Discrepancy is a way of assessing how far is a discrete (normalized) counting measure supported in $[0,1)^d$ from the uniform distribution on $[0,1)^d$. Apart from being interesting in its own rights it also connects to numerical integration via Koksma-Hlawka type inequalities. Given a finite point set $P \subset [0,1)^d$ with cardinality $N$, its *local discrepancy* at the point $x \in [0,1)^d$, denoted $D(P,x)$, is given by

$$D(P,x) := \left| \frac{|P \cap Q_x|}{N} - \lambda^d(Q_x) \right|, \tag{2.1}$$

where $Q_x$ is a box anchored at 0, i.e. a $d$-dimensional interval $[0,x)$. This definition corresponds to the intuition that if the point set $P$ is "almost uniformly" distributed then the fraction of points from $P$ falling into $Q_x$ should not be far away from $\lambda^d(Q_x)$. That is, a small discrepancy is seen as an indicator that the point set $P$ is close to being uniformly distributed.

For a fixed $P$ one may consider $D(P,\cdot)$ as a function defined on $[0,1)^d$. One is interested in different $L^p$-norms of $D(P,\cdot)$. Arguably the most interesting is the case $p = \infty$. Via

$$D^*(P) := \|D(P,\cdot)\|_\infty$$

one defines the *star discrepancy* of the point set $P$. However, also different norms are frequently used. Generally for $p \geq 1$ one may define the *$L^p$-discrepancy* by $D^p(P) := \|D(P,\cdot)\|_p$.

Sometimes to highlight the cardinality of the underlying point set $P$ we denote the local discrepancy by $D_N(P,x)$ and the star discrepancy by $D_N^*(P)$.

**Remark 2.3.1.** A natural generalization of the classical discrepancy would be the following. Let $(X,\Sigma,\mu)$ be a probability space and $\mathcal{S} \subset \Sigma$ some class of measurable subsets of $X$. For a finite point set $P \subset X$with cardinality $N$ and $S \in \mathcal{S}$ we define the local discrepancy of $P$ in $S$ by

$$D_{X,\mathcal{S}}(P,S) = \left| \frac{|P \cap S|}{N} - \mu(S) \right|.$$

Let now $(\mathcal{S},\Sigma',\nu)$ be a further probability space. For $p \geq 1$ one may define the $L^p$-discrepancy of $P$ with respect to $\nu$ via $D^p_{X,\mathcal{S},\nu}(P) = \|D_{X,\mathcal{S}}(P,\cdot)\|_{L^p(\nu)}$.

### 2.3.1 Discrepancy and Numerical Integration

Relevance of the discrepancy theory for numerical integration comes from the so called Koksma-Hlawka type inequalities, which relate the QMC-Integration error in different function spaces obtained using a given point set $P$ as integration nodes, with the discrepancy of $P$. One of the Koksma-Hlawka inequalities is the following: let $f : [0,1)^d \to \mathbb{R}$ have finite Hardy-Krause variation $V_{\mathrm{HK}}(f)$. Given a point set $P$ with $N$ elements it holds

$$\left| \frac{1}{N} \sum_{p \in P} f(p) - \int_{[0,1)^d} f(x)\, dx \right| \leq V_{\mathrm{HK}}(f) D^*(P).$$

Moreover, the inequality is sharp in the sense that for every point set $P$ and $\epsilon > 0$ there exists a function $f : [0,1)^d \to \mathbb{R}$ with $V_{\mathrm{HK}}(f) = 1$ and

$$\left| \frac{1}{N} \sum_{p \in P} f(p) - \int_{[0,1)^d} f(x)\, dx \right| > D^*(P) - \epsilon,$$

see [79]. Koksma-Hlawka type inequalities are interesting amongst other things since they enable us to give upper bounds on the integration error in terms of two factors, one of which depends only on the function at hand and the other only on the quality of the point set used as integration nodes.

For more information on this subject see [126, 123, 103, 59] and a monograph [85].

### 2.3.2 Asymptotic and Preasymptotic Bounds on Minimal Discrepancy

The basic question in discrepancy theory is: how fast does the minimal (star, $L^p$) disrepancy of point sets $P_N$ with $|P_N| = N$ converge to 0 as $N$ converges to $\infty$? To be more precise define the *minimal star discrepancy of N points* by

$$D_N^* := \inf_{P_N \subset [0,1)^d, |P_N| = N} D^*(P_N).$$

Analogously one may define the minimal $L^p$-discrepancy. Here we give a short overview of historical results on this problem. We start with the asymptotic point of view, meaning that we are considering the dependence of discrepancy only on the number of points, but the dimension of the space stays fixed.

In 1954 Klaus Roth showed that in all dimensions $d \geq 2$ there exists a constant $c_d > 0$ depending only on $d$ such that $D_N^* \geq c_d \frac{\log(N)^{\frac{d-1}{2}}}{N}$, see [98]. In fact he proved a lower bound on $D_N^2$ and then used the obvious relation $D_N^* \geq D_N^2$. More then twenty years later, in [100], Wolfgang Schmidt generalized Roth's result to the case of $L^p$-discrepancy, proving that there exists a constant $c_{d,p} > 0$ depending only on $d$ and $p$ for which $D_N^p \geq c_{d,p} \frac{\log(N)^{\frac{d-1}{2}}}{N}$. Schmidt showed also a sharp bound on the minimal star discrepancy in dimension $d = 2$ by proving that in this case there exists a constant $c > 0$ such that $D_N^* \geq \frac{\log(N)}{N}$, see [99]. Roth's and Schmidt's theorems are up till now almost the best known results. Apart from Jozsef Beck's new bound in dimension $d = 3$ ([7]) the first bigger progress has been obtained by D. Bilyk, M. Lacey and A. Vagharshakyan, who showed ([8],[9]) that for $d \geq 3$ there exists $\eta(d) > 0$ such that $D_N^* \geq \frac{\log(N)^{\frac{d-1}{2}+\eta(d)}}{N}$. So far no better lower bound in dimension $d \geq 3$ are known.

The best known asymptotic upper bounds on the minimal discrepancy for $d \geq 2$ are of the form $D_N^* \leq C_d \frac{\log(N)^{d-1}}{N}$. They have been shown by van der Corput in dimension $d = 2$ (see [113, 114]) and extended by Halton to higher dimensions ([52]). Those upper bounds on discrepancy are constructive, i.e. one shows that a concrete sequence of point sets obeys them. Point sets for which those upper bound hold are known as low-discrepancy point

sets. Today many constructions of low-discrepancy point sets (e.g. digital $(0, m, d)$-nets) are known.

There are at least two reasons, why the asymptotic bounds on discrepancy are not satisfactory from the practitioner's point of view. First of all, the dependence on the dimension $d$ is hidden in the implicit constant. Secondly, the bounds indeed apply only in the asymptotic regime. To see this note that for the function $N \mapsto \frac{\log(N)^{d-1}}{N}$ to be decreasing one needs $N \geq e^{d-1}$ which, as a number of points is prohibitive even for moderate $d$. To overcome those problems one tries to establish the so-called preasymptotic bounds on $D_N^*$, i.e. bounds with explicit dependence on $N$ as well as on $d$.

It has been shown by Hinrichs in [61] that there exist constants $c, \epsilon_0 > 0$ such that $D_N^* \geq \min\left\{\epsilon_0, c\frac{d}{N}\right\}$.

Concerning the upper bounds in the preasymptotic regime, in 2001 in [57] it was proved that for some (implicit) constant $C > 0$ it holds $D_N^* \leq C\sqrt{\frac{d}{N}}$. The first reasonably small upper bound on $C$ has been given by Aistlaitner in [2]. Combining the probabilistic method with the so-called dyadic chaining he argued that $C \leq 9.65$. Further refinement of the probabilistic method led to showing that in fact $C < 2.53$, see [41].

There is still a big gap between the lower and the upper preasymptotic bounds on the minimal star discrepancy. Closing it is seen as one of the most important and challenging probems of the discrepancy theory.

# Chapter 3

# Explicit Error Bounds for Randomized Smolyak Algorithms and an Application to Infinite-dimensional Integration

## 3.1 Introduction

Smolyak's method or algorithm, also known as sparse grid method, Boolean method, combination technique or discrete blending method, was outlined by Smolyak in [104]. It is a general method to treat multivariate tensor product problems. Its major advantage is the following: to tackle a multivariate tensor product problem at hand one only has to understand the corresponding univariate problem. More precisely, Smolyak's algorithm uses algorithms for the corresponding univariate problem as building blocks, and it is fully determined by the choice of those algorithms. If those algorithms for the univariate problem are optimal, then typically Smolyak's algorithm for the multivariate problem is almost optimal, i.e., its convergence rate is optimal up to logarithmic factors.

Today Smolyak's method is widely used in scientific computing and there exists a huge number of scientific articles dealing with applications and modifications of it. A partial list of papers (which is, of course, very far from being complete) on *deterministic Smolyak algorithms* may contain, e.g., the articles [116, 117] for general approximation problems, [31, 13, 107, 6, 28, 83, 32, 33, 96, 44, 51] for numerical integration, [48, 12, 106, 108, 101, 112, 24] for function recovery, and [95, 127, 82, 124, 125, 29, 30] for other applications. Additional references and further information may be found in the survey articles [11, 49], the book chapters [85, Chapter 15], [109, Chapter 4], and the books [14, 25].

On *randomized Smolyak algorithms* much less is known. Actually, we are only aware of two articles that deal with randomized versions of Smolyak's method, namely [19] and [56]. In [19] Dick et al. investigate a specific instance of the randomized Smolyak method and use it as a tool to show that higher order nets may be used to construct integration algorithms achieving almost optimal order of convergence (up to logarithmic

factors) of the worst case error in certain Sobolev spaces. In [56] Heinrich and Milla employ the randomized Smolyak method as a building block of an algorithm to compute antiderivatives of functions from $L^p([0,1]^d)$ allowing for fast computation of antiderivative values for any point in $[0,1]^d$. Note that in both cases the randomized Smolyak method is applied as an ad hoc device and none of the papers gives a systematic treatment of its properties.

Here we want to start a systematic treatment of randomized Smolyak algorithms. Similar to the paper [116], where the deterministic Smolyak method was studied, we discuss the randomized Smolyak method for general linear approximation problems on tensor products of Hilbert spaces. Examples of such approximation problems are numerical integration and $L^2$-approximation, i.e., function recovery.

The error criteria for randomized algorithms or, more generally, randomized operators that we consider are extensions of the worst case error for deterministic algorithms. The first error criterion is the randomized root mean square error, sometimes referred to as "randomized error". This error criterion is typically used to assess the quality of randomized algorithms. The second error criterion is the root mean square worst case error, sometimes referred to as "worst case error". This quantity is commonly used to prove the existence of a good *deterministic* algorithm with the help of the "pidgeon hole principle": It arises as an average of the usual deterministic worst case error over a set of deterministic algorithms $\mathcal{A}$ endowed with a probability measure $\mu$. If the average is small, there exists at least one algorithm in $\mathcal{A}$ with small worst case error, see, e.g., [19] or [103]. Notice that the pair $(\mathcal{A}, \mu)$ can be canonically identified with a randomized algorithm.

We derive upper error bounds for both error criteria for randomized Smolyak algorithms with explicitly given dependence on the number of variables and the number of information evaluations used. The former number is the underlying dimension of the problem, the latter number is typically proportional to the cost of the algorithm. The upper error bounds show that the randomized Smolyak method can be efficiently used at least in moderately high dimension. We complement this result by providing lower error bounds for randomized Smolyak algorithms that nearly match our upper bounds.

As in the deterministic case, our upper and lower error bounds contain logarithmic factors whose powers depend linearly on the underlying dimension $d$, indicating that the direct use of the randomized Smolyak method in very high dimension may be prohibitive. Nevertheless, our upper error bound shows that randomized Smolyak algorithms make perfect building blocks for more sophisticated algorithms such as multilevel algorithms (see, e.g., [54, 58, 34, 35, 36, 60, 81, 39, 40, 5, 15, 67]), multivariate decomposition methods (see, e.g., [68, 97, 115, 40, 15, 16]) or dimension-wise quadrature methods (see [50]). We demonstrate this in the case of the infinite-dimensional integration problem on weighted tensor products of reproducing kernel Hilbert spaces with general kernels. We provide the exact polynomial convergence rate of $N$-th minimal errors—the corresponding upper error bound is established by multivariate decomposition methods based on randomized Smolyak algorithms.

The chapter is organized as follows: In Section 3.2 we provide a general multivariate problem formulation and illustrate it with two examples. In Section 3.3 we introduce a

randomized multivariate Smolyak method building on randomized univariate algorithms. Our assumptions about the univariate randomized algorithms resemble the ones made in [116] in the deterministic case. In Remark 3.3.2 we observe that we may identify our randomized linear approximation problem of interest with a corresponding deterministic $L^2$-approximation problem.

In Section 3.4 we follow the course of [116] and establish first error bounds in terms of the underlying dimension of the problem and the level of the considered Smolyak algorithm, see Theorem 3.4.1 and Corollary 3.4.2. For the randomized error criterion Remark 3.3.2 helps us to boil down the error analysis of the randomized Smolyak method to the error analysis of the deterministic Smolyak method provided in [116]. For the root mean square worst case error criterion Remark 3.3.2 is of no help and therefore we state the details of the analysis (which, nevertheless, adapts the proof technique from [116, Lemma 2]).

Up to this point we consider general randomized operators to approximate the solution we are seeking for. In Section 3.5 we focus on randomized algorithms and the information evaluations they use. In Theorem 3.5.4 we present upper error bounds for the randomized Smolyak method where the dependence on the underlying dimension of the problem and on the number of information evaluations is revealed. In Corollary 3.5.12 we provide lower error bounds for the randomized Smolyak method.

In Section 3.6 we apply our upper error bounds for randomized Smolyak algorithms to the infinite-dimensional integration problem. After introducing the setting, we provide the exact polynomial convergence rate of $N$-th minimal errors in Theorem 3.6.5. In Corollary 3.6.6 we compare the power of randomized algorithms and deterministic algorithms for infinite-dimensional integration, and in Corollary 3.6.7 we illustrate the result of Theorem 3.6.5 for weighted Korobov spaces. In Remark 3.6.8 and Remark 3.6.9 we discuss previous contributions to the considered infinite-dimensional integration problem and generalizations to other settings such as function spaces with increasing smoothness or the $L^2$-approximation problem.

## 3.2 Formulation of the Problem

Let $d \in \mathbb{N}$. For $n = 1, \dots, d$, let $F^{(n)}$ be a separable Hilbert space of real valued functions, $G^{(n)}$ be a separable Hilbert space, and $S^{(n)} : F^{(n)} \to G^{(n)}$ be a continuous linear operator. We consider now the tensor product spaces $F_d$ and $G_d$ given by

$$F_d := F^{(1)} \otimes \cdots \otimes F^{(d)},$$

$$G_d := G^{(1)} \otimes \cdots \otimes G^{(d)},$$

and the tensor product operator $S_d$ (called *solution operator*) given by

$$S_d := S^{(1)} \otimes \cdots \otimes S^{(d)}.$$

We frequently use results concerning tensor products of Hilbert spaces and tensor product operators without giving explicit reference, for details on this subject see, e.g., Section

2.1 and references therein. We denote the norms in $F^{(n)}$ and $F_d$ by $\|\cdot\|_{F^{(n)}}$ and $\|\cdot\|_{F_d}$ respectively, and the norms in $G^{(n)}$ and $G_d$ simply by $\|\cdot\|$. Furthermore, $L(F_d, G_d)$ denotes the space of all bounded linear operators between $F_d$ and $G_d$ endowed with the standard operator norm $\|\cdot\|_{\mathrm{op}}$ induced by the norms on $F_d$ and $G_d$.

$S_d(f)$ may be approximated by randomized linear algorithms or, more generally, by randomized linear operators.

**Definition 3.2.1.** Let $(\Omega, \Sigma, \mathbf{P})$ be a probability space, $F$ be a separable Hilbert space of real-valued functions, and $G$ be a separable Hilbert space.

A *randomized linear operator* $A$ is a mapping

$$A : \Omega \to L(F, G)$$

such that $Af : \Omega \to G$ is a random variable for each $f \in F$; here $G$ is endowed with its Borel $\sigma-$field.

We put

$$\mathcal{O}^{\mathrm{ran}} := \mathcal{O}^{\mathrm{ran,lin}}(\Omega, F_d, G_d) := \{A : \Omega \to L(F_d, G_d) \mid A \text{ is a randomized linear operator}\}.$$

Obviously one may interpret deterministic bounded linear operators as randomized linear operators with trivial dependance on $\Omega$. Accordingly, we put

$$\mathcal{O}^{\mathrm{det}} := \mathcal{O}^{\mathrm{det,lin}}(F_d, G_d) := L(F_d, G_d) \subset \mathcal{O}^{\mathrm{ran,lin}}(\Omega, F_d, G_d),$$

where the inclusion is based on the identification of $A \in L(F_d, G_d)$ with the constant mapping $\Omega \ni \omega \mapsto A$.

**Definition 3.2.2.** A *(randomized) linear approximation problem* is given by a quadruple $\{S, F, G, \mathcal{O}(\Omega)\}$, where $F$ is a separable Hilbert space of real-valued functions, $G$ is a separable Hilbert space, $S : F \to G$ is the solution operator, and $\mathcal{O}(\Omega) \subseteq \mathcal{O}^{\mathrm{ran,lin}}(\Omega, F, G)$ denotes the class of admissible randomized linear operators.

We are mainly interested in results for randomized linear algorithms, which constitute a subclass of $\mathcal{O}^{\mathrm{ran}}$ and will be introduced in Section 3.5.

Let $A$ be a randomized linear operator that approximates the solution operator $S$.

**Definition 3.2.3.** Consider the randomized linear approximation problem $(S, F, G, \mathcal{O}(\Omega))$. The *randomized error* (or: randomized root mean square error) of the operator $A \in \mathcal{O}(\Omega)$ is given by

$$e^{\mathrm{r}}(A) := e^{\mathrm{r}}(S, A) := \sup_{\|f\|_F \le 1} \left[\mathbf{E}\|(S - A)f\|^2\right]^{\frac{1}{2}}, \tag{3.1}$$

and the *root mean square (RMS) worst case error* (or: randomized worst case error) is given by

$$e^{\mathrm{w}}(A) := e^{\mathrm{w}}(S, A) := \left[\mathbf{E} \sup_{\|f\|_F \le 1} \|(S - A)f\|^2\right]^{\frac{1}{2}}. \tag{3.2}$$

Clearly we have $0 \le e^{\mathrm{r}}(S,A) \le e^{\mathrm{w}}(S,A)$.

Notice that for a *deterministic* linear operator $A$ both errors coincide with the *deterministic worst case error*

$$e^{\mathrm{d}}(A) := e^{\mathrm{d}}(S,A) := \sup_{\|f\|_{F_d} \le 1} \|(S-A)f\|,$$

i.e., $e^{\mathrm{d}}(S,A) = e^{\mathrm{r}}(S,A) = e^{\mathrm{w}}(S,A)$.

We finish this section by giving two examples of typical tensor product problems that fit into the framework given above.

**Example 3.2.4.** *For $n = 1, \dots, d$, let $D^{(n)} \neq \emptyset$ be an arbitrary domain and let $\rho^{(n)}$ be a positive measure on $D^{(n)}$. Denote by $E$ the Cartesian product $D^{(1)} \times \cdots \times D^{(d)}$ and by $\mu$ the product measure $\otimes_{n=1}^{d} \rho^{(n)}$ on $E$.*

(*i*) *By choosing $F^{(n)} \subset L^2(D^{(n)}, \rho^{(n)})$, $G^{(n)} := \mathbb{R}$, and $S^{(n)}$ to be the integration functional $S^{(n)}(f) = \int_{D^{(n)}} f \,\mathrm{d}\rho^{(n)}$, we obtain $F_d \subset L^2(E,\mu)$, $G_d = \mathbb{R}$, and $S_d$ is the integration functional on $F_d$ given by*

$$S_d(f) = \int_E f \,\mathrm{d}\mu, \qquad f \in F_d.$$

*The* integration problem *is now to compute or approximate for given $f \in F_d$ the integral $S_d(f)$.*

(*ii*) *By choosing $F^{(n)} \subset G^{(n)} := L^2(D^{(n)}, \rho^{(n)})$ and $S^{(n)}$ to be the embedding operator from $F^{(n)}$ into $G^{(n)}$, we obtain $F_d \subset G_d = L^2(E,\mu)$ and $S_d$ is the embedding operator from $F_d$ into $G_d$ given by*

$$S_d(f) = f, \qquad f \in F_d.$$

*The* $L^2$-approximation problem *is now to reconstruct a given function $f \in F_d$, i.e., to compute or approximate $S_d(f)$; the reconstruction error is measured in the $L^2$-norm.*

*Note that in both problem formulations above the phrase "a given function $f$" does not necessarilly mean that the whole function is known. Usually there is only partial information about the function available (like a finite number of values of the function or of its derivatives or a finite number of Fourier coefficients). We discuss this point in more detail in Section 3.5.1.*

## 3.3 Smolyak Method for Tensor Product Problems

From now on we are interested in randomizing the Smolyak method which is to be defined in this section. Assume that for every $n = 1, 2, \dots, d$, we have a sequence of randomized linear operators $(U_l^{(n)})_{l \in \mathbb{N}}$, which approximate the operator $S^{(n)}$, such that for every $f \in$

$F^{(n)}$ it holds: $U_l^{(n)} f$ is a random variable on a probability space $(\Omega^{(n)}, \Sigma^{(n)}, \mathbf{P}^{(n)})$. We shall refer to separate $U_l^{(n)}$ as to *building blocks*.

Put $\Omega := \Omega^{(1)} \times \ldots \times \Omega^{(d)}, \Sigma := \bigotimes_{n=1}^d \Sigma^{(n)}, \mathbf{P} := \bigotimes_{n=1}^d \mathbf{P}^{(n)}$. We denote

$$\Delta_0^{(n)} := U_0^{(n)} := 0, \quad \Delta_l^{(n)} := U_l^{(n)} - U_{l-1}^{(n)}, \quad l \in \mathbb{N},$$

and

$$Q(L,d) := \left\{ \mathbf{l} \in \mathbb{N}^d \,|\, \|\mathbf{l}\|_1 \leq L \right\}.$$

Note that if $L \geq d$, then $|Q(L,d)| = \binom{L}{d}$.

**Definition 3.3.1.** Consider the linear tensor product approximation problem $\{S_d, F_d, G_d, \mathcal{O}(\Omega)\}$ as defined in Section 3.2. The *randomized (d-dimensional) Smolyak method (of level $L$)*, is given for every $f \in F_d$ by

$$A(L,d)f : \Omega \to G_d, \quad \omega \mapsto \left( \sum_{\mathbf{l} \in Q(L,d)} \bigotimes_{n=1}^d \Delta_{l_n}^{(n)}(\omega_n) \right) f. \tag{3.3}$$

We would like to stress that due to the definition of the probability space $(\Omega, \Sigma, \mathbf{P})$ for given $f_n \in F^{(n)}, n = 1, 2, \ldots, d$, the families $((U_l^{(n)} f_n)_{l \in \mathbb{N}}), n = 1, 2, \ldots, d$, are mutually independent. Note that for $L < d$ the Smolyak method is the zero operator. Therefore, we will always assume (without stating it explicitly every time) that $L \geq d$.

It can be verified that the following representation holds

$$A(L,d) = \sum_{L-d+1 \leq |\mathbf{l}| \leq L} (-1)^{L-|\mathbf{l}|} \binom{d-1}{L-|\mathbf{l}|} \bigotimes_{n=1}^d U_{l_n}^{(n)}, \tag{3.4}$$

cf. [116, Lemma 1]. When investigating the randomized error we need that for every $l \in \mathbb{N}$ and $n = 1, \ldots, d$,

$$U_l^{(n)} f \in L^2(\Omega^{(n)}, G^{(n)}) \quad \text{for all } f \in F^{(n)}. \tag{3.5}$$

In the RMS worst case error analysis we require for every $l \in \mathbb{N}$ and $n = 1, \ldots, d$,

$$\tau_{l,n}(\omega) := \sup_{\|f\|_{F^{(n)}} \leq 1} \|(U_l^{(n)} f)(\omega_n)\| < \infty \quad \text{for all } \omega_n \in \Omega^{(n)}, \tag{3.6}$$

and that $\tau_{l,n} : \Omega \to [0, \infty)$ is measurable with

$$\|\tau_{l,n}\|_{L^2(\Omega^{(n)}, \mathbb{R})} < \infty. \tag{3.7}$$

Let $\mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}$. When considering the error $e^{\mathrm{x}}(S_d, A(L,d))$, we assume that there exist constants $B, C, E > 0$ and $D \in (0,1)$ such that for every $n = 1, 2, \ldots, d$, and every $l \in \mathbb{N}$

$$\|S^{(n)}\|_{\mathrm{op}} \leq B, \tag{3.8}$$

$$e^{\mathrm{x}}(S^{(n)}, U_l^{(n)}) \leq CD^l, \tag{3.9}$$

and additionally if x = r

$$\sup_{\|f\|_{F^{(n)}}\leq 1} \left[ \mathbf{E} \|\underbrace{U_l^{(n)} f - U_{l-1}^{(n)} f}_{=\Delta_l^{(n)} f}\|^2 \right]^{\frac{1}{2}} \leq ED^l, \tag{3.10}$$

and if x = w

$$\left[ \mathbf{E} \sup_{\|f\|_{F^{(n)}}\leq 1} \|\underbrace{U_l^{(n)} f - U_{l-1}^{(n)} f}_{=\Delta_l^{(n)} f}\|^2 \right]^{\frac{1}{2}} \leq ED^l. \tag{3.11}$$

Note that (3.9) implies the conditions (3.10) and (3.11) with a constant $E := C(1 + D^{-1})$ for all $l \geq 2$. Still (3.10) and (3.11) may even hold for some smaller $E$.

Note furthermore that our assumptions (3.8) to (3.11) resemble the assumptions made in [116, Sect. 4.1] for the analysis of deterministic Smolyak algorithms.

**Remark 3.3.2.** For our randomized error analysis it would be convenient to identify a randomized linear operator $A : \Omega \to L(F, G)$, $F, G$ separable Hilbert spaces, with the mapping (3.12) which we again denote by $A$ :

$$A : F \to L^2(\Omega, G), \quad f \mapsto \big(\omega \mapsto Af(\omega)\big). \tag{3.12}$$

We now show that this identification makes sense for all the operators we are considering. We start with the building blocks $U_l^{(n)}$. From (3.10) we obtain

$$\sup_{\|f\|_{F^{(n)}}\leq 1} \left[\mathbf{E}\|U_l^{(n)} f\|^2\right]^{1/2} \leq \frac{ED}{1-D}, \tag{3.13}$$

implying $(U_l^{(n)} f)(\cdot) \in L^2(\Omega^{(n)}, G^{(n)})$ for all $f \in F^{(n)}$. The building blocks $U_l^{(n)}$ are obviously linear as mappings $F^{(n)} \to L^2(\Omega^{(n)}, G^{(n)})$ and, due to (3.13), also bounded, i.e. continuous. Now, since for arbitrary sample spaces $\Omega_1, \Omega_2$ and separable Hilbert spaces $H_1, H_2$ it holds

$$L^2(\Omega_1, H_1) \otimes L^2(\Omega_2, H_2) \cong L^2(\Omega_1 \times \Omega_2, H_1 \otimes H_2),$$

we have, due to the assumed product structure of the probability space $(\Omega, \Sigma, \mathbf{P})$ (reflecting the mutual independence of the families of randomized algorithms $(U_l^{(n)})_{l\in\mathbb{N}}$, $n = 1, 2, \ldots, n$) that $(\bigotimes_{n=1}^d U_{l_n}^{(n)})(f)(\cdot)$ lies in $L^2(\Omega, G_d)$ for $f \in F_d$. Clearly, the tensor product operator $\bigotimes_{n=1}^d U_{l_n}^{(n)}$ is a bounded linear mapping $F_d \to L^2(\Omega, G_d)$. Since due

to (3.4) the Smolyak method $A(L,d)$ may be represented as a finite sum of such tensor product operators, it is also a bounded linear mapping $F_d \to L^2(\Omega, G_d)$.

If we formally consider $S_d$ as an operator $F_d \to L^2(\Omega, G_d)$, $f \mapsto \big(\omega \mapsto S_d f\big)$ (i.e., an operator that maps into the constant $L^2$-functions), then $S_d$ is still linear and continuous with operator norm

$$\|S_d\|_{\mathrm{op}} = \sup_{\|f\|_{F_d}\leq 1} \|S_d f\|_{L^2(\Omega,G)} = \sup_{\|f\|_{F_d}\leq 1} \mathbf{E}\left[\|S_d f(\omega)\|^2\right]^{1/2},$$

and the usual randomized error can be written as

$$e^{\mathrm{r}}(S_d, A) = \sup_{\|f\|_{F_d}\leq 1} \|(S_d - A)f\|_{L^2(\Omega,G_d)} = \|S_d - A\|_{\mathrm{op}}. \tag{3.14}$$

The RMS worst case error unfortunately does not allow for a representation as operator norm similar to (3.14).

Note that the above identification turns a randomized approximation problem

$$S : F \to G, \quad A : \Omega \to L(F,G)$$

into a deterministic $L^2$-approximation problem

$$S : F \to L^2(\Omega, G), \quad A : F \to L^2(\Omega, G).$$

## 3.4 Error Analysis in Terms of the Level

We now perform the error analysis of the approximation of $S_d$ by the Smolyak method $A(L,d)$ in terms of the level $L$, which may be done under the rather general assumptions of Sections 3.2 and 3.3.

**Theorem 3.4.1.** *For $L, d \in \mathbb{N}, L \geq d$ let $A(L,d)$ be a randomized Smolyak method as in Definition 3.3.1. Let $\mathrm{x} \in \{\mathrm{w}, \mathrm{r}\}$. Assume* (3.8), (3.9) *and, dependently on the setting, for $\mathrm{x} = \mathrm{r}$ additionally assume (3.5),(3.10) and for $\mathrm{x} = \mathrm{w}$ additionally assume (3.6), (3.7) and* (3.11). *Then we have*

$$e^{\mathrm{x}}(S_d, A(L,d)) \leq C B^{d-1} D^{L-d+1} \sum_{j=0}^{d-1} \left(\frac{ED}{B}\right)^j \binom{L-d+j}{j} \leq C H^{d-1} \binom{L}{d-1} D^L, \tag{3.15}$$

*where $H = \max\{\frac{B}{D}, E\}$.*

The form of the error bound (3.15) for both randomized error criteria is the same as the form of the error bound for the worst case error of deterministic Smolyak algorithms presented in [116, Lemma 2]. Indeed, in our proof we adapt the proof strategy from [116, Lemma 2] from the deterministic to the randomized setting.

In the deterministic case it is known that under more specific assumptions on the underlying spaces and the solution operator one may get even an asymptotically stronger error bound, where the factor $\binom{L}{d-1}$ is essentially replaced by $\sqrt{\binom{L}{d-1}}$, see, e.g., [44]. Similar phenomenon may be seen also in the randomized setting, cf. Chapter 4, in particular Theorem 4.2.11.

*Proof of Theorem 3.4.1.* As already pointed out in the proof of [116, Lemma 2], the second inequality in (3.15) follows easily by using $\sum_{j=0}^{d-1}\binom{L-d+j}{j}=\binom{L}{d-1}$ and estimating $(\frac{ED}{B})^j \leq \max\{1,(\frac{ED}{B})^{d-1}\}$, so all there remains to be done is proving the first inequality.

Firstly we shall focus on the RMS worst case error bound. Note that for a fixed $\omega\in\Omega$

$$\sup_{\|f\|_{F_d}\leq 1}\|(S_d-A(L,d)(\omega))f\|^2=\left(\sup_{\|f\|_{F_d}\leq 1}\|(S_d-A(L,d)(\omega))f\|\right)^2=\|S_d-A(L,d)(\omega)\|_{\mathrm{op}}^2$$

Now we may proceed similarly as in the proof of Lemma 2 from [116], by induction on $d,L$ for $d\in\mathbb{N}$ and $L\in\{d,d+1,\ldots\}$. For $d=1$ and any $L\in\mathbb{N}$ we have $S_d=S^{(1)}$ and $A(L,1)=U_L^{(1)}$, so the statement is just the condition (3.9). Suppose we have already proved the claim for $L,d$ and want to prove it for $L+1,d+1$. Using

$$A(L+1,d+1)=\sum_{\mathbf{l}\in Q(L,d)}\bigotimes_{n=1}^{d}\Delta_{l_n}^{(n)}\otimes U_{L+1-|\mathbf{l}|}^{(d+1)}$$

and Minkowski's inequality we get

$$\begin{aligned}
&e^{\mathrm{w}}(S_{d+1},A(L+1,d+1))=\left[\mathbf{E}\|S_{d+1}-A(L+1,d+1)\|_{\mathrm{op}}^2\right]^{\frac{1}{2}}\\
&=\left[\mathbf{E}\|\sum_{\mathbf{l}\in Q(L,d)}(\bigotimes_{n=1}^{d}\Delta_{l_n}^{(n)})\otimes(S^{(d+1)}-U_{L+1-|\mathbf{l}|}^{(d+1)})+(S_d-A(L,d))\otimes S^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}}\\
&\leq\left[\mathbf{E}\|\sum_{\mathbf{l}\in Q(L,d)}(\bigotimes_{n=1}^{d}\Delta_{l_n}^{(n)})\otimes(S^{(d+1)}-U_{L+1-|\mathbf{l}|}^{(d+1)})\|_{\mathrm{op}}^2\right]^{\frac{1}{2}}+\left[\mathbf{E}\|(S_d-A(L,d))\otimes S^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}}.
\end{aligned}$$

We use Minkowski's inequality, properties of tensor product operator norms, the fact that component algorithms $U_l^{(n)},l\in\mathbb{N}$ are randomized independently for different

$n \in \{1, \dots, d\}$, (3.9) and (3.11) to obtain

$$\begin{aligned}
&\left[\mathbf{E}\| \sum_{\mathbf{l}\in Q(L,d)} (\bigotimes_{n=1}^{d} \Delta_{l_n}^{(n)}) \otimes (S^{(d+1)} - U_{L+1-|\mathbf{l}|}^{(d+1)})\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} \\
&\leq \sum_{\mathbf{l}\in Q(L,d)} \left[\mathbf{E}\| \bigotimes_{n=1}^{d} \Delta_{l_n}^{(n)}\|_{\mathrm{op}}^2 \|S^{(d+1)} - U_{L+1-|\mathbf{l}|}^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} \\
&= \sum_{\mathbf{l}\in Q(L,d)} \left(\prod_{n=1}^{d} \left[\mathbf{E}\|\Delta_{l_n}^{(n)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}}\right) \left[\mathbf{E}\|S^{(d+1)} - U_{L+1-|\mathbf{l}|}^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} \\
&\leq \sum_{\mathbf{l}\in Q(L,d)} CE^d D^{L+1} = \binom{L}{d} CE^d D^{L+1}.
\end{aligned}$$

Furthermore, using (3.8),

$$\begin{aligned}
\mathbf{E}\left[\|(S_d - A(L,d)) \otimes S^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} &= \mathbf{E}\left[\|(S_d - A(L,d))\|_{\mathrm{op}}^2 \|S^{(d+1)}\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} \\
&= \|S^{(d+1)}\|_{\mathrm{op}} \, \mathbf{E}\left[\|(S_d - A(L,d))\|_{\mathrm{op}}^2\right]^{\frac{1}{2}} \\
&\leq Be^{\mathrm{w}}(S_d, A(L,d)).
\end{aligned}$$

Therefore we have

$$e^{\mathrm{w}}(S_{d+1}, A(L+1, d+1)) \leq \binom{L}{d} E^d C D^{L+1} + Be^{\mathrm{w}}(S_d, A(L,d))$$

and using the induction hypothesis finishes the proof for the RMS worst case error.

Now consider the randomized error. By similar calculations as in the first part of the proof one could show that the claim holds true for the randomized error for elementary tensors. Then however, one encounters problems trying to lift it to the whole Hilbert space. The main difficulty lies in the fact that the randomized error is not an operator norm of a suitable sum of tensor product operators mapping $F_d$ into $G_d$, which would have enabled us to bound it by a sum of products of norms of the corresponding univariate operators which has proved to be useful in bounding the deterministic worst case error, see [116]. To get around it we need a different approach. A remedy is to interpret a randomized problem as a deterministic $L^2-$approximation problem. As already explained in Remark 3.3.2 we may identify $(S_d - A(L,d)) : \Omega \to L(F_d, G_d)$ with an operator $F_d \to L^2(\Omega, G_d)$ again denoted by $(S_d - A(L,d))$. Recall that the mutual independence of the families of randomized algorithms $(U_l^{(n)})_{l\in\mathbb{N}}$, $n = 1, 2, \dots, d$, is crucial to make this identification work. Then however $e^{\mathrm{r}}(S_d, A(L,d)) = \|S_d - A(L,d)\|_{\mathrm{op}}$ and we may proceed exactly as in the proof of [116, Lemma 2], which finishes the proof of Theorem 3.4.1. □

We may generalize the result of Theorem 3.4.1 by allowing for more flexibility in convergence rates in (3.9), (3.10) and (3.11). This generalization can be used to capture

additional logarithmic factors in the error bounds for the building block algorithms. This turns out to be particularly useful when investigating the error bounds for Smolyak methods whose building blocks are, e.g., multivariate quadratures or approximation algorithms, as it is the case in [19]. Suppose namely that there exist a constant $D \in (0,1)$ and non decreasing sequences of positive numbers $(C_l)_l, (E_l)_l, l \in \mathbb{N}$, such that for every $l \in \mathbb{N}$

$$e^{\mathrm{x}}(S^{(n)}, U_l^{(n)}) \leq C_l D^l, \quad \mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}. \tag{3.16}$$

Moreover, if $\mathrm{x} = \mathrm{r}$

$$\sup_{\|f\|_{F^{(n)}} \leq 1} \left[ \mathbf{E} \| \underbrace{U_l^{(n)} f - U_{l-1}^{(n)} f}_{=\Delta_l^{(n)} f} \|^2 \right]^{\frac{1}{2}} \leq E_l D^l, \tag{3.17}$$

and if $\mathrm{x} = \mathrm{w}$

$$\left[ \mathbf{E} \sup_{\|f\|_{F^{(n)}} \leq 1} \| \underbrace{U_l^{(n)} f - U_{l-1}^{(n)} f}_{=\Delta_l^{(n)} f} \|^2 \right]^{\frac{1}{2}} \leq E_l D^l. \tag{3.18}$$

It is now easy to prove Corollary 3.4.2 along the lines of the proof of Theorem 3.4.1.

**Corollary 3.4.2.** *For $L, d \in \mathbb{N}, L \geq d$ let $A(L,d)$ be a randomized Smolyak method as described in Section 3.3. Let $\mathrm{x} \in \{\mathrm{w}, \mathrm{r}\}$. Assume* (3.8)*,* (3.16) *and, dependently on the setting, for $\mathrm{x} = \mathrm{r}$ assume (3.5),(3.17) and for $\mathrm{x} = \mathrm{w}$ assume (3.6), (3.7) and* (3.18)*. Then we have*

$$e^{\mathrm{x}}(S_d, A(L,d)) \leq C_L B^{d-1} D^{L-d+1} \sum_{j=0}^{d-1} \left( \frac{E_{L-1} D}{B} \right)^j \binom{L-d+j}{j} \leq C_L H_L^{d-1} \binom{L}{d-1} D^L, \tag{3.19}$$

*where $H_L = \max\{\frac{B}{D}, E_{L-1}\}$.*

**Remark 3.4.3.** Note that applying Corollary 3.4.2 to the uni- or multivariate building block algorithms error bounds from [19] we may reproduce the error bounds obtained in that paper for the final (higher-dimensional) Smolyak method.

## 3.5 Error Analysis in Terms of Information

### 3.5.1 Algorithms

Consider a linear approximation problem $\{S, F, G, \mathcal{O}(\Omega)\}$. The aim of this section is to specify those linear operators that we want to call algorithms and to explain the typical information-based complexity framework for investigating the error of an algorithm in terms of the cardinality of information, for further reference see, e.g., [110]. To this end we shall specify a class of linear bounded functionals on $F$ called *admissible information*

*functionals* and denoted by $\Lambda$, which will become one more parameter of the approximation problem. Given a constant $\tau \in \mathbb{N}_0$ and, if $\tau > 0$, a collection of functionals $\lambda_i \in \Lambda, i = 1, \dots, \tau$, the *information operator* $\mathcal{N} : F \to \mathbb{R}^{\max\{\tau,1\}}$ applied to $f \in F$ is determined via

$$\mathcal{N}(f) = \begin{cases} 0 & \text{if } \tau = 0, \\ (\lambda_1(f), \dots, \lambda_\tau(f)) & \text{else.} \end{cases}$$

Note that we are considering only non-adaptive information, meaning that the information functionals used do not depend on $f \in F$.

**Definition 3.5.1.** A deterministic linear operator $A \in \mathcal{O}^{\mathrm{det,lin}}(F, G)$ is called a *deterministic linear algorithm* if it admits a representation

$$A = \phi \circ \mathcal{N},$$

where $\mathcal{N}$ is an information operator and $\phi : \mathbb{R}^{\max\{\tau,1\}} \to G$ is an arbitrary mapping.

We denote the number of information functionals used by the deterministic algorithm $A$ for any input $f \in F$ by $\mathrm{card}^{\mathrm{det}}(A, F)$, i.e.,

$$\mathrm{card}^{\mathrm{det}}(A, F) := \tau.$$

We denote the class of deterministic linear algorithms with admissible information functionals $\Lambda$ by $\mathcal{A}^{\mathrm{det,lin}}(F, G, \Lambda)$.

Let $(V_l)_{l\in\mathbb{N}}$ be an arbitrary sequence of algorithms and let $(\lambda_{l,i})_{i\in[m_l]}$ be the information functionals used by $V_l$. We say that the sequence $(V_l)_l$ *uses nested information* if for every $a < b$

$$\{\lambda_{a,i} \,|\, i \in [m_a]\} \subseteq \{\lambda_{b,i} \,|\, i \in [m_b]\}.$$

**Definition 3.5.2.** A mapping $A \in \mathcal{O}^{\mathrm{ran,lin}}(\Omega, F, G)$ is called a *randomized linear algorithm* if the range of $A$ is $\mathcal{A}^{\mathrm{det,lin}}(F, G, \Lambda)$ for some class of functionals $\Lambda$ and $\omega \mapsto \mathrm{card}^{\mathrm{det}}(A(\omega), F)$ is a random variable.

We denote the class of randomized linear algorithms with admissible information functionals $\Lambda$ by $\mathcal{A}^{\mathrm{ran,lin}}(\Omega, F, G, \Lambda) =: \mathcal{A}(\Omega, \Lambda)$.

For a randomized linear algorithm $A$ we may finally define

$$\mathrm{card}^{\mathrm{ran}}(A, F) := \mathbf{E}\left[\mathrm{card}^{\mathrm{det}}(A, F)\right].$$

We say that the information used by a sequence of randomized linear algorithms is *nested* if it is nested for almost every $\omega \in \Omega$. Note that the information used by $(A(L, d))_{L\geq d}$ is nested.

**Example 3.5.3.** *Consider the integration problem from Example 3.2.4. Let $s \in \mathbb{N}$. For $n = 1, \dots, d$, let $D^{(n)} = [0, 1)^s$, $\rho^{(n)}$ be the Lebesgue measure on $[0, 1)^s$ and $F^{(n)}$ be some reproducing kernel Hilbert space of functions defined on $[0, 1)^s$ (e.g., a Sobolev space with sufficiently high smoothness parameter).*

*Choose a prime number $b \geq s$. For $n = 1, \ldots, d$, and $l \in \mathbb{N}$ let $\mathcal{P}_l^{(n)}$ be a scrambled $(0, l, s)-$net in base $b$ as introduced in [90]. Now*

$$U_l^{(n)} : F^{(n)} \to \mathbb{R}, \quad f \mapsto \frac{1}{b^l} \sum_{x \in \mathcal{P}_l^{(n)}} f(x)$$

*is a randomized algorithm. Moreover, if we randomize $(U_l^{(n)})_{n,l}$ in such a way that the families $(U_l^{(n)})_l$ are independent then we may use them as building blocks of the Smolyak method and all the results of this section apply, in specific cases cf. also [19] and Chapter 4.*

Now we would like to make some reasonable assumptions on the cost of building blocks of the Smolyak method. Consider a randomized Smolyak method as described in Section 3.3 with building blocks being randomized algorithms. Let

$$m_{l,n} := \mathrm{card}^{\mathrm{ran}}(U_l^{(n)}, F^{(n)}).$$

Notice that $m_{0,n} = 0$. For $d \in \mathbb{N}, L = d, d+1, \ldots$ put

$$N := N(L, d) := \mathrm{card}^{\mathrm{ran}}(A(L, d), F_d).$$

Let us assume that there exist constants $1 \leq K_{\mathrm{low}} \leq K_{\mathrm{up}}, 1 < K$ such that for every $n = 1, \ldots, d, l \in \mathbb{N}$ it holds

$$K_{\mathrm{low}} K^{l-1}(K-1) \leq m_{l,n} - m_{l-1,n} \leq K_{\mathrm{up}} K^{l-1}(K-1). \tag{3.20}$$

Note that this implies

$$K_{\mathrm{low}}(K^l - 1) \leq m_{l,n} \leq K_{\mathrm{up}}(K^l - 1), \quad l \in \mathbb{N}. \tag{3.21}$$

### 3.5.2 Upper Error Bounds

Throughout the whole section we require that the assumptions of Theorem 3.4.1 hold. Let us define

$$\alpha := \frac{\log(\frac{1}{D})}{\log(K)}, \tag{3.22}$$

where $K$ is as in (3.20) and $D$ is as in (3.9). We define the *polynomial convergence rate of the algorithms $U_l^{(n)}, l \in \mathbb{N}$*, by

$$\mu_{\mathrm{x}}^{(n)} := \sup\{\delta \geq 0 \mid \sup_{l \in \mathbb{N}} e^{\mathrm{x}}(S^{(n)}, U_l^{(n)}) m_{l,n}^{\delta} < \infty\} \tag{3.23}$$

where $\mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}$. It is straightforward to verify that $\alpha \leq \mu_{\mathrm{x}}^{(n)}$ for every $n$. Indeed,we have

$$e^{\mathrm{x}}(S^{(n)}, U_l^{(n)}) \leq \frac{C K_{\mathrm{up}}^{\alpha}}{m_{l,n}^{\alpha}}, \tag{3.24}$$

because of

$$\frac{CK_{\mathrm{up}}^{\alpha}}{m_{l,n}^{\alpha}} \geq \frac{CK_{\mathrm{up}}^{\alpha}}{K_{\mathrm{up}}^{\alpha}(K^l-1)^{\alpha}} \geq \frac{C}{K^{l\alpha}} = CD^l. \tag{3.25}$$

Hence for each $n \in \{1,\dots,d\}$ the quantity $\alpha$ is a lower bound on the polynomial order of convergence $\mu_{\mathrm{x}}^{(n)}$ of the algorithms $U_l^{(n)}, l \in \mathbb{N}$, and can be chosen arbitrarily close to $\mu_{\mathrm{x}}^{(n)}$ if the constants $C$ and $D$ in (3.9) are chosen appropriately.

The aim of this section is to develop upper bounds on the error of $d-$variate Smolyak method in terms of $N, d$ and $\alpha$. More concretely we prove the following theorem.

**Theorem 3.5.4.** *Let* $\mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}$. *Let* $K_{\mathrm{low}}, K_{\mathrm{up}}, K$ *be as in (3.20),* $\alpha$ *as in* (3.22) *and let the assumptions of Theorem 3.4.1 hold. Then there exist constants* $C_0, C_1$ *such that for all* $d \in \mathbb{N}$ *and all* $L \geq d$ *it holds*

$$e^{\mathrm{x}}(A(L,1)) \leq C_0 C_1 N^{-\alpha} \tag{3.26}$$

*and*

$$e^{\mathrm{x}}(A(L,d)) \leq C_0 C_1^d \left(1 + \frac{\log(N)}{d-1}\right)^{(d-1)(\alpha+1)} N^{-\alpha}, \ d \geq 2, \tag{3.27}$$

*where* $N = N(L,d)$ *is the cardinality of information used by the algorithm* $A(L,d)$.

As already indicated after Theorem 3.4.1, it may be possible to improve the upper error bound (3.27) for more specific Hilbert spaces and solution operators. For numerical integration on certain wavelet spaces for instance, the authors were able to reduce the power $(d-1)(\alpha+1)$ of the logarithmic factor to $(d-1)(\alpha+1/2)$, see Chapter 4. This phenomenon also appears in the deterministic setting, cf. [44].

To prove Theorem 3.5.4 we need a lemma bounding $N(L,d)$ in terms of $K_{\mathrm{low}}, K_{\mathrm{up}}, K, d$ and $L$. Notice that the function $x \mapsto \left(1 + \frac{\log(x)}{d-1}\right)^{(d-1)(\alpha+1)} x^{-\alpha}$ is not monotone decreasing but unimodal. That is why we also need lower bound for $N(L,d)$.

**Lemma 3.5.5.** *Let* $K_{\mathrm{low}}, K_{\mathrm{up}}, K$ *be as in* (3.20). *Put*

$$N_l^{\mathrm{nest}} := N_l^{\mathrm{nest}}(L,d) = K_{\mathrm{low}}^d \left(\frac{K-1}{K}\right)^d K^L \binom{L-1}{d-1},$$

$$N_u := N_u(L,d) = K_{\mathrm{up}}^d \frac{K}{K-1} K^L \binom{L-1}{d-1},$$

$$N_u^{\mathrm{nest}} := N_u^{\mathrm{nest}}(L,d) := K_{\mathrm{up}}^d \left(\frac{K-1}{K}\right)^d K^L \binom{L-1}{d-1}.$$

*For every* $d \in \mathbb{N}$ *and* $L \geq d$ *it holds*

$$N_l^{\mathrm{nest}}(L,d) \leq N(L,d) \leq N_u(L,d).$$

*Moreover, if the building blocks of the Smolyak method use nested information then*

$$N_l^{\mathrm{nest}}(L,d) \leq N(L,d) \leq N_u^{\mathrm{nest}}(L,d).$$

Notice that the upper bounds on $N(L,d)$ in Lemma 3.5.5 are the same as the ones obtained in [116, Lemma 7] in the deterministic case.

*Proof.* Due to (3.4) we have

$$\begin{aligned}
N(L,d) &= \mathbf{E}\left[\mathrm{card}^{\mathrm{det}}\left(\sum_{L-d+1\leq|\mathbf{l}|\leq L}(-1)^{L-|\mathbf{l}|}\binom{d-1}{L-|\mathbf{l}|}\bigotimes_{n=1}^{d}U_{l_n}^{(n)}(\omega)\right)\right]\\
&\leq \sum_{L-d+1\leq|\mathbf{l}|\leq L}\mathbf{E}\left[\mathrm{card}^{\mathrm{det}}\left(\bigotimes_{n=1}^{d}U_{l_n}^{(n)}(\omega)\right)\right]\\
&= \sum_{L-d+1\leq|\mathbf{l}|\leq L}\prod_{n=1}^{d}\mathbf{E}\left[\mathrm{card}^{\mathrm{det}}\left(U_{l_n}^{(n)}(\omega)\right)\right]\\
&= \sum_{L-d+1\leq|\mathbf{l}|\leq L}\prod_{n=1}^{d}m_{l_n,n}\leq K_{\mathrm{up}}^{d}\sum_{L-d+1\leq|\mathbf{l}|\leq L}K^{|\mathbf{l}|}.
\end{aligned}$$

Now following the steps of [116, Lemma 7] we obtain

$$\begin{aligned}
N(L,d) &\leq K_{\mathrm{up}}^{d}\sum_{|\mathbf{l}|=L-d+1}^{L}K^{|\mathbf{l}|}\leq K_{\mathrm{up}}^{d}\sum_{\nu=L-d+1}^{L}K^{\nu}\binom{\nu-1}{d-1}\\
&\leq K_{\mathrm{up}}^{d}\binom{L-1}{d-1}(K^{L+1}-K^{L-d+1})(K-1)^{-1}\\
&\leq K_{\mathrm{up}}^{d}\frac{K}{K-1}K^{L}\binom{L-1}{d-1}=N_u.
\end{aligned}$$

Now we provide a lower bound on $N(L,d)$. Note that given the cardinality of information used by the building blocks, the cardinality of information used by the Smolyak method is minimal when the information used by the building blocks is nested for every coordinate. In this case the information used by the Smolyak method is exactly the information used by $\sum_{|\mathbf{l}|=L}\bigotimes_{n=1}^{d}U_{l_n}^{(n)}$. Let us fix $\mathbf{l}\in\mathbb{N}^d, |\mathbf{l}|=L$. The expected value of the cardinality of information used by $\bigotimes_{n=1}^{d}U_{l_n}^{(n)}$ and at the same time not used by any other $\bigotimes_{n=1}^{d}U_{v_n}^{(n)}$ with $|\mathbf{v}|=L$ is

$$\prod_{n=1}^{d}(m_{l_n,n}-m_{l_n-1,n})\geq K_{\mathrm{low}}^{d}K^{L-d}(K-1)^{d}. \tag{3.28}$$

We obtain

$$\begin{aligned}
N(L,d) &\geq \sum_{|\mathbf{l}|=L}K_{\mathrm{low}}^{d}K^{L-d}(K-1)^{d}\\
&= K_{\mathrm{low}}^{d}\left(\frac{K-1}{K}\right)^{d}K^{L}\binom{L-1}{d-1}=N_l^{\mathrm{nest}}.
\end{aligned}$$

The upper bound in the case when the building blocks use nested information follows in exactly the same manner on noting that

$$K_{\mathrm{up}}^d K^{L-d}(K-1)^d \geq \prod_{n=1}^{d}(m_{l_n,n} - m_{l_n-1,n}), \tag{3.29}$$

cf. also the discussion in [116, p. 26]. □

**Example 3.5.6.** *Let $b \in \mathbb{N}_{\geq 2}$. Suppose that for every $n = 1, \ldots, d, l \in \mathbb{N}$ the cardinality of information used by $U_l^{(n)}$ is $b^l$. This is e.g. the case if the building blocks are quadratures such that $U_l^{(n)}$ is based on a $(0, l, s)$-net in base $b$. Then (3.20) is satisfied with $K = b, K_{\mathrm{low}} = 1, K_{\mathrm{up}} = 2$. Now we may easily see from Lemma 3.5.5 that the cardinality of information used by the Smolyak method $A(L, d)$ based on those building blocks is $\Theta(b^L L^{d-1})$.*

*Proof of Theorem 3.5.4.* Note that $N(L, 1) = m_{L,1}$ so we have already showed the statement for $d = 1$ in (3.25). It remains to consider the case $d > 1$. Consider the function

$$f : [1, \infty) \to \mathbb{R}, \quad x \mapsto \left(1 + \frac{\log(x)}{d-1}\right)^{(d-1)(\alpha+1)} x^{-\alpha}.$$

We will show that there exist constants $\widetilde{C}_{u,0}, \widetilde{C}_{u,1}, \widetilde{C}_{l,0}, \widetilde{C}_{l,1}$, such that for $N_u, N_l$ from Lemma 3.5.5 it holds

$$e^{\mathrm{x}}(A(L, d)) \leq \widetilde{C}_{u,0}\widetilde{C}_{u,1}^d f(N_u) \tag{3.30}$$

and

$$e^{\mathrm{x}}(A(L, d)) \leq \widetilde{C}_{l,0}\widetilde{C}_{l,1}^d f(N_l). \tag{3.31}$$

Now unimodality of $f$ combined with the fact that the extremum is a maximum yields $f(N(L, d)) \geq \min\{f(N_u), f(N_l)\}$, finishing the proof.

First we prove (3.30). Calling upon Theorem 3.4.1 and using $L \leq \frac{\log(N_u)}{\log(K)}$ we get

$$\begin{aligned}
e^{\mathrm{x}}(A(L, d)) &\leq CH^{d-1}\binom{L}{d-1}D^L \\
&= CH^{d-1}\binom{L}{d-1}K^{-L\alpha} \\
&= CH^{d-1}\binom{L}{d-1}\left(K_{\mathrm{up}}^d \frac{K}{K-1}\right)^{\alpha}\binom{L-1}{d-1}^{\alpha} N_u^{-\alpha} \\
&\leq \frac{C}{H}(HK_{\mathrm{up}}^{\alpha})^d \left(\frac{K}{K-1}\right)^{\alpha}\binom{L}{d-1}^{\alpha+1} N_u^{-\alpha} \\
&\leq \frac{C}{H}(HK_{\mathrm{up}}^{\alpha})^d \left(\frac{K}{K-1}\right)^{\alpha} \frac{\log(N_u)^{(d-1)(\alpha+1)}}{(\log(K))^{(d-1)(\alpha+1)}((d-1)!)^{\alpha+1}} N_u^{-\alpha} \\
&= \frac{C}{((d-1)!)^{\alpha+1}H}\left(\frac{K\log(K)}{K-1}\right)^{\alpha}\log(K)\left(\frac{HK_{\mathrm{up}}^{\alpha}}{(\log(K))^{\alpha+1}}\right)^d \frac{\log(N_u)^{(d-1)(\alpha+1)}}{N_u^{\alpha}}
\end{aligned}$$

$$= ((d-1)!)^{-\alpha-1} C_{u,0} C_{u,1}^d \frac{\log(N_u)^{(d-1)(\alpha+1)}}{N_u^\alpha},$$

with constants $C_{u,0}, C_{u,1}$ not depending neither on $d$ nor on $N(L,d)$. By Stirling's formula we conclude

$$\begin{aligned} e^{\mathrm{x}}(A(L,d)) &\leq \left( \frac{e^d}{(2\pi)^{\frac{1}{2}}(d-1)^{\frac{1}{2}}(d-1)^{(d-1)}} \right)^{\alpha+1} C_{u,0} C_{u,1}^d \frac{\log(N_u)^{(d-1)(\alpha+1)}}{N_u^\alpha} \\ &\leq \widetilde{C}_{u,0} \widetilde{C}_{u,1}^d \left( \frac{\log(N_u)}{d-1} \right)^{(d-1)(\alpha+1)} N_u^{-\alpha}. \end{aligned}$$

Now we prove (3.31). To this end it suffices to prove that there exist constants $\hat{C}_0, \hat{C}_1$ independent of $d$ and $N$ such that

$$\left( \frac{\log(N_u)}{d-1} \right)^{(d-1)(\alpha+1)} N_u^{-\alpha} \leq \hat{C}_0 \hat{C}_1^d \left( 1 + \frac{\log(N_l)}{d-1} \right)^{(d-1)(\alpha+1)} N_l^{-\alpha}, \tag{3.32}$$

i.e.,

$$\left( \frac{N_l}{N_u} \right)^\alpha \left( \frac{\log(N_u)}{(d-1)+\log(N_l)} \right)^{(d-1)(\alpha+1)} \leq \hat{C}_0 \hat{C}_1^d.$$

Note that

$$\frac{N_u}{N_l} = \left( \frac{K}{K-1} \right)^{d+1} \left( \frac{K_{\mathrm{up}}}{K_{\mathrm{low}}} \right)^d$$

so, putting $\hat{K} = \frac{K}{K-1} \frac{K_{\mathrm{up}}}{K_{\mathrm{low}}}$ we have

$$\begin{aligned} \frac{\log(N_u)}{(d-1)+\log(N_l)} \leq & \frac{\log\left(\frac{K}{K-1}\right) + d\log(\hat{K}) + \log(N_l)}{(d-1)+\log(N_l)} \\ & \leq \log\left(\frac{K}{K-1}\right) + \frac{d}{d-1}\log(\hat{K}) + 1 \leq \log\left(\frac{K}{K-1}\right) + 2\log(\hat{K}) + 1. \end{aligned}$$

Since obviously $\left(\frac{N_l}{N_u}\right)^\alpha \leq 1$ this shows (3.32) and finishes the proof of the theorem. □

### 3.5.3 Lower Error Bounds

Lower error bounds for rather specific applications of the Smolyak method in the determinisic setting may be found e.g. in [101]. Our aim here is to introduce simple and general lower bounds in the randomized setting.

In this subsection we make the following additional assumptions.

The first assumption states that there exist a sequence of instances of the problem $\{S_d, F_d, G_d, \mathcal{A}(\Omega,\Lambda)\}$ that is genuinely univariate, i.e., there exists a sequence $(f_l)_{l\in\mathbb{N}} \in F_d$, $f_l = g_{1,l} \otimes g_{2,l} \otimes \cdots \otimes g_{d,l}$ such that $\|f_l\|_{F_d} = 1$ for which

$$\|(S^{(2)} \otimes \cdots \otimes S^{(d)})(g_{2,l} \otimes \cdots \otimes g_{d,l})\| =: \theta_d > 0, \tag{3.33}$$

and the $U_l^{(n)}, l \geq 1$, are exact on $g_{n,l}$ for $n > 1$ .

Secondly, we assume that there exist constants $\widetilde{C} > 0, \widetilde{D} \in (0,1)$ such that for every $l \in \mathbb{N}$

$$\left[ \mathbf{E} \| S^{(1)} g_{1,l} - U_l^{(1)} g_{1,l} \|^2 \right]^{\frac{1}{2}} \geq \widetilde{C} \widetilde{D}^l. \tag{3.34}$$

Let us put

$$\beta := \frac{\log(\frac{1}{\widetilde{D}})}{\log(K)},$$

with $\widetilde{D}$ as in (3.34) and $K$ as in (3.20). Using (3.34) and (3.21) one easily sees that

$$\left[ \mathbf{E} \| (S^{(1)} - U_l^{(1)}) g_{1,l} \|^2 \right]^{\frac{1}{2}} \geq \widetilde{C} \left( K_{\text{low}} (1 - K^{-1}) \right)^{\beta} m_{l,1}^{-\beta}, \tag{3.35}$$

meaning that we have $\beta \geq \mu_{\text{x}}^{(1)}$, where $\mu_{\text{x}}^{(1)}$ is the polynomial convergence rate of $(U_l^{(1)})_{l \in \mathbb{N}}$ as defined in (3.23). Moreover, by choosing $(g_{1,l})_{l \in \mathbb{N}}, \widetilde{C}, \widetilde{D}$ appropriately, $\beta$ can be made arbitrarily close to $\mu_{\text{x}}^{(1)}$.

**Example 3.5.7.** *The assumptions made in this subsection are quite naturally met for many important problems. Consider for instance an integration problem as described in Example 3.2.4, where $F^{(n)}, n = 2, \ldots, d$, may be any spaces containing constant functions. Then, for an appropriate $(g_{1,l})_{l \in \mathbb{N}}$ (chosen so that the integration error does not converge too fast to 0) we have that*

$$f_l := g_{1,l} \otimes \mathbf{1}_D \otimes \cdots \otimes \mathbf{1}_D, \quad l \in \mathbb{N},$$

*satisfies our assumptions for any randomized quadrature with weights adding up to 1.*

**Lemma 3.5.8.** *Let $\text{x} \in \{\text{w}, \text{r}\}$, and let (3.33) and (3.34) hold. Then there exists a constant $\hat{c}_d$ such that*

$$e^{\text{x}}(A(L,d)) \geq \hat{c}_d m_{L,1}^{-\beta}$$

*for all $L \geq d$.*

*If additionally (3.33) and (3.34) are satisfied for all $d \in \mathbb{N}$ with the same constants $\widetilde{C}$ and $\widetilde{D}$ and $\Theta := \sup_{L,d} \left( \frac{m_{L,1}}{m_{L-d+1,1}} \right)^{2\beta} \theta_d^2$ is bounded, then we may choose the constants $(\hat{c}_d)_{d \in \mathbb{N}}$ in such a way that they are all equal.*

*Proof.* Choosing $f_l$ satisfying (3.33), due to exactness assumption we obtain

$$\begin{aligned} A(L,d) f_l &= \sum_{\mathbf{l} \in Q(L,d)} \bigotimes_{n=1}^{d} \Delta_{l_n}^{(n)} f_{n,l} \\ &= \sum_{t=1}^{L-d+1} \Delta_t^{(1)} g_{1,l} \otimes \Delta_1^{(2)} g_{2,l} \cdots \otimes \Delta_1^{(d)} g_{d,l} \\ &= U_{L-d+1}^{(1)} g_{1,l} \otimes S^{(2)} g_{2,l} \cdots \otimes S^{(d)} g_{d,l}. \end{aligned}$$

Let us put $T := \bigotimes_{n=2}^{d} S^{(n)}, h = \bigotimes_{n=2}^{d} g_{n,l}$. Due to (3.35) we have

$$\begin{aligned} e^{\mathrm{x}}(A(L,d))^2 &\geq \mathbf{E}\|(S_d - A(L,d))f_l\|^2 = \mathbf{E}\|(S^{(1)} \otimes T - U^{(1)}_{L-d+1} \otimes T)f_l\|^2 \\ &= \mathbf{E}\|(S^{(1)} - U^{(1)}_{L-d+1})g_{1,l} \otimes Th\|^2 = \|Th\|^2 \, \mathbf{E}\|(S^{(1)} - U^{(1)}_{L-d+1})g_{1,l}\|^2 \\ &= \theta_d^2 \, \mathbf{E}\|(S^{(1)} - U^{(1)}_{L-d+1})g_{1,l}\|^2 \geq \widetilde{C}^2 \theta_d^2 \left(K_{\mathrm{low}}(1 - K^{-1})\right)^{2\beta} \left(\frac{m_{L,1}}{m_{L-d+1,1}}\right)^{2\beta} m_{L,1}^{-2\beta}. \end{aligned}$$

□

**Remark 3.5.9.** In particular constants $(\hat{c}_d)_{d\in\mathbb{N}}$ may be chosen all equal e.g. when (3.33) and (3.34) are satisfied for all $d \in \mathbb{N}$ with the same constants $\widetilde{C}, \widetilde{D}$ and $\theta := \sup_{d\in\mathbb{N}} \theta_d < \infty$.

**Lemma 3.5.10.** *Let there exist constants $1 \leq K_{\mathrm{low}} \leq K_{\mathrm{up}}, 1 < K$ such that for all $n = 1, \ldots, d$ and $l \in \mathbb{N}$ (3.20) is satisfied. Then there exists a constant $\widetilde{c}_d$ such that*

$$\widetilde{c}_d m_{L,1} (\log(m_{L,1}))^{d-1} \leq N(L,d)$$

*for all $L \geq d$. Moreover, if $\xi := \xi(d) := (K^d - 1)^{\frac{1}{d}} > 1$ then there exists a constant $\widetilde{C}_d$ such that*

$$N(L,d) \leq \widetilde{C}_d m_{L,1} (\log(m_{L,1}))^{(d-1)}$$

*for all $L \geq d$.*

*Proof.* First we prove the upper bound.

On the one hand, due to (3.21) it holds

$$\begin{aligned} m_{L,1} \log(m_{L,1})^{d-1} &\geq K_{\mathrm{low}} \frac{K^L - 1}{K^L} \log(K_{\mathrm{low}}(K^L - 1))^{d-1} K^L \\ &\geq K_{\mathrm{low}} \frac{K^d - 1}{K^d} \log\left(\left[(K_{\mathrm{low}}(K^L - 1))^{\frac{1}{L}}\right]^L\right)^{d-1} K^L \\ &\geq K_{\mathrm{low}} \frac{K^d - 1}{K^d} \log(\xi)^{d-1} L^{d-1} K^L, \end{aligned}$$

where we used that the function $[0, \infty) \ni x \mapsto (K^x - 1)^{\frac{1}{x}}$ is increasing.

On the other hand, according to Lemma 3.5.5

$$N(L,d) \leq K_{\mathrm{up}}^d \frac{K}{K-1} \binom{L-1}{d-1} K^L \leq K_{\mathrm{up}}^d \frac{K}{K-1} \frac{1}{(d-1)!} L^{d-1} K^L.$$

It follows that the constant

$$\widetilde{C}_d = K_{\mathrm{up}}^d \frac{K}{K-1} \frac{1}{(d-1)!} \left[K_{\mathrm{low}} \frac{K^d - 1}{K^d} \log(\xi)^{d-1}\right]^{-1}$$

does the job.

Now we prove the lower bound.

On the one hand due to (3.21) we have

$$m_{L,1}(\log(m_{L,1}))^{d-1} \leq K_{\mathrm{up}}(K^L-1)\left(\log(K_{\mathrm{up}}(K^L-1))\right)^{d-1} \leq K_{\mathrm{up}}\left(\log(K_{\mathrm{up}}^{\frac{1}{L}}K)\right)^{d-1}K^L L^{d-1}.$$

Noticing that $f:[d,\infty)\to\mathbb{R}, x\mapsto \frac{(x-1)\cdots(x-d+1)}{x^{d-1}}$ is increasing we obtain

$$\begin{aligned}\binom{L-1}{d-1} &= \frac{(L-1)\cdots(L-d+1)}{L^{d-1}}\frac{L^{d-1}}{(d-1)!} \geq \frac{(d-1)!}{d^{d-1}}\frac{L^{d-1}}{(d-1)!}\\ &= \frac{1}{d^{d-1}}L^{d-1}.\end{aligned}$$

On the other hand we have due to Lemma 3.5.5

$$\begin{aligned}N(L,d) &\geq \left(\frac{(K-1)K_{\mathrm{low}}}{K}\right)^d K^L\binom{L-1}{d-1}\\ &\geq \left(\frac{(K-1)K_{\mathrm{low}}}{K}\right)^d \frac{1}{d^{d-1}}K^L L^{d-1}.\end{aligned}$$

It follows that the constant

$$\widetilde{c}_d = \left(\frac{(K-1)K_{\mathrm{low}}}{K}\right)^d \frac{1}{d^{d-1}}\left(K_{\mathrm{up}}\left(\log(K_{\mathrm{up}}^{\frac{1}{d}}K)\right)^{d-1}\right)^{-1}$$

satisfies

$$\widetilde{c}_d m_{L,1}(\log(m_{L,1}))^{(d-1)} \leq N(L,d).$$

□

**Remark 3.5.11.** Note that the constants $\widetilde{C}_d$ and $\widetilde{c}_d$ from Lemma 3.5.10 fall superexponentially fast in $d$.

**Corollary 3.5.12.** *Let* $\mathrm{x}\in\{\mathrm{r},\mathrm{w}\}$. *Let (3.33) and (3.34) hold. Furthermore, let there exist constants* $1\leq K_{\mathrm{low}}\leq K_{\mathrm{up}}, 1<K$ *such that for all* $n=1,\dots,d$, *and* $l\in\mathbb{N}$ *(3.20) is satisfied. Moreover, assume that* $m_{L,1}\geq 16$. *Then there exists a constant* $c_d$ *such that given* $\delta\in(0,1)$ *there exists* $N(\delta)$ *such that for every* $N\geq N(\delta)$

$$e^{\mathrm{x}}(A(L,d)) \geq c_d\frac{(\log(N))^{(d-1-\delta)\beta}}{N^\beta}$$

*with* $\beta=\frac{\log(\frac{1}{D})}{\log(K)}$ *and* $N=N(L,d)$.

*Proof.* Let $\widetilde{c}$ be such that for every $L\in\mathbb{N}$

$$\widetilde{c}m_{L,1}(\log(m_{L,1}))^{d-1} \leq N(L,d).$$

The existence of $\widetilde{c}$ is guaranteed by Lemma 3.5.10. We put $\widetilde{c}_0 := \min\{\widetilde{c},1\}$.

We would like to express the bound from Lemma 3.5.8 in terms of the cardinality $N := N(L,d)$. To this end we want to find a function $g : \mathbb{R} \to \mathbb{R}$ of the form $g(x) = \frac{x^\beta}{(\log(x))^\eta}$ such that for large $m$

$$g(m(\log(m))^{d-1}) \geq m^\beta \tag{3.36}$$

implying

$$e^{\mathrm{x}}(A(L,d)) \geq \frac{\hat{c}_d}{m_{L,1}^\beta} \geq \frac{\hat{c}_d}{g(m_{L,1}(\log(m_{L,1}))^{d-1})}.$$

We rewrite (3.36) as

$$\frac{m^\beta(\log(m))^{(d-1)\beta}}{(\log(m(\log(m))^{d-1}))^\eta} \geq m^\beta.$$

Hence (3.36) holds if

$$\eta \leq \frac{(d-1)\beta\log(\log(m))}{\log\left(\log(m) + (d-1)\log(\log(m))\right)}$$

and the expression on the right hand side converges from below to $(d-1)\beta$ as $m$ goes to $\infty$. To obtain

$$\frac{\hat{c}_d}{g(m_{L,1}\log(m_{L,1})^{d-1})} \geq \frac{\hat{c}_d}{g(\widetilde{c}_0^{-1}N)}$$

it is sufficient to check that g is increasing on the interval $[m_{L,1}\log(m_{L,1})^{d-1}, \infty)$. Simple calculations reveal that $g$ is increasing on $[e^{\frac{\eta}{\beta}}, \infty) \supset [e^{d-1}, \infty)$. The final step is to notice that

$$e^{\mathrm{x}}(A(L,d)) \geq \frac{\hat{c}_d}{g(\widetilde{c}_0^{-1}N)} = \hat{c}_d\frac{\log(\widetilde{c}_0^{-1}N)^\eta}{(\widetilde{c}_0^{-1}N)^\beta} \geq \hat{c}_d\widetilde{c}_0^\beta\frac{\log(N)^\eta}{N^\beta}.$$

Putting $c_d := \hat{c}_d\widetilde{c}_0^\beta$ finishes the proof. □

## 3.6 Application to Infinite-Dimensional Integration

In Theorem 3.6.5 we provide a sharp result on randomized infinite-dimensional integration on weighted reproducing kernel Hilbert spaces that parallels the sharp result on deterministic infinite-dimensional integration stated in [42, Theorem 5.1]. Results from [40] and from [97] in combination with Theorem 3.5.4 rigorously establish the sharp randomized result in the special case where the weighted reproducing kernel Hilbert space is based on an anchored univariate kernel. With the help of the embedding tools provided in [42] this result will be extended to general weighted reproducing kernel Hilbert spaces. Before we can state and prove Theorem 3.6.5 we first have to introduce the setting, cf. [42].

For basic results about reproducing kernels $K$ and the corresponding Hilbert spaces $H(K)$ we refer to Section 2.2 and references therein. We denote the norm on $H(K)$ by $\|\cdot\|_K$ and the space of constant functions (on a given domain) by $H(1)$; here 1 denotes the constant kernel that only takes the function value one.

### 3.6.1 Assumptions

Henceforth we assume that

(A1) $H$ is a vector space of real-valued functions on a domain $D \neq \emptyset$ with $H(1) \subsetneq H$

and

(A2) $\|\cdot\|_1$ and $\|\cdot\|_2$ are seminorms on $H$, induced by symmetric bilinear forms $\langle\cdot,\cdot\rangle_1$ and $\langle\cdot,\cdot\rangle_2$, such that $\|1\|_1 = 1$ and $\|1\|_2 = 0$.

Let

$$\|f\|_H := \left(\|f\|_1^2 + \|f\|_2^2\right)^{1/2} \quad \text{for } f \in H. \tag{3.37}$$

Furthermore, we assume that

(A3) $\|\cdot\|_H$ is a norm on $H$ that turns this space into a reproducing kernel Hilbert space, and there exists a constant $c \geq 1$ such that

$$\|f\|_H \leq c\left(|\langle f, 1\rangle_1| + \|f\|_2\right) \quad \text{for all } f \in H. \tag{3.38}$$

Condition (3.38) is equivalent to the fact that $\|\cdot\|_H$ and $|\langle\cdot,1\rangle_1| + \|\cdot\|_2$ are equivalent norms on $H$.

Let us restate Lemma 2.1 from [42]:

**Lemma 3.6.1.** *For each $\gamma > 0$ there exists a uniquely determined reproducing kernel $k_\gamma$ on $D \times D$ such that $H(1 + k_\gamma) = H$ as vector spaces and*

$$\|f\|_{1+k_\gamma}^2 = \|f\|_1^2 + \frac{1}{\gamma}\|f\|_2^2.$$

*Moreover, the norms $\|\cdot\|_H$ and $\|\cdot\|_{1+k_\gamma}$ are equivalent and $H(1) \cap H(k_\gamma) = \{0\}$.*

Note that for the special value $\gamma = 1$ we have $\|\cdot\|_{1+k_1} = \|\cdot\|_H$.

The next example illustrates the assumptions and the statement of Lemma 3.6.1; for more information and a slight generalization see [42, Example 2.3], cf. also Example 2.2.4.

**Example 3.6.2.** *Let $D := [0,1)$ and $r > 1/2$. The* Korobov space $K_r = K_r([0,1))$ *(also known as* periodic Sobolev space, see, e.g., [101]*) is the Hilbert space of all $f \in L^2([0,1))$ with finite norm*

$$\|f\|_r^2 := |\hat{f}(0)|^2 + \sum_{h \in \mathbb{Z}\setminus\{0\}} |\hat{f}(h)|^2 h^{2r},$$

*where $\hat{f}(h) = \int_0^1 f(t)e^{-2\pi i h t}\,\mathrm{d}t$ is the $h$-th Fourier coefficient of $f$. The notation we use here, following [84], is a little bit unconventional. In many sources $r$ is replaced by $\frac{r}{2}$. The functions in $K_r$ are continuous and periodic. It is easily checked that the reproducing kernel of $K_r$ is given by*

$$1 + k_1(x,y) = 1 + \sum_{h \in \mathbb{Z}\setminus\{0\}} h^{-2r} e^{2\pi i h(x-y)}, \quad x, y \in [0,1). \tag{3.39}$$

*Consider the pair of seminorms on $K_r$ given by*

$$\|f\|_1 = |\hat{f}(0)| \quad \text{and} \quad \|f\|_2^2 = \sum_{h\neq 0} |\hat{f}(h)|^2\, h^{2r}.$$

*The assumptions (A1), (A2), and (A3) are easily verified. For $\gamma > 0$ we have $k_\gamma = \gamma \cdot k_1$.*

Further examples of spaces that satisfy the assumptions (A1), (A2), and (A3) are, for instance, the *(non-periodic) Sobolev spaces* $W^{r,2}([0,1))$ of smoothness $r \in \mathbb{N}$ endowed with either the standard norm, the anchored norm or the ANOVA norm, see [42, Example 2.1].

We now want to study weighted tensor product Hilbert spaces of multivariate functions, which implies that we have to consider *product weights* as introduced in [103]. More precisely, we consider a sequence $\boldsymbol{\gamma} = (\gamma_j)_{j\in\mathbb{N}}$ of positive weights that satisfies

$$\sum_{j=1}^{\infty} \gamma_j < \infty. \tag{3.40}$$

The decay of the weights is quantified by

$$\operatorname{decay}(\boldsymbol{\gamma}) := \sup\Big(\Big\{p > 0 \,\Big|\, \sum_{j=1}^{\infty} \gamma_j^{1/p} < \infty\Big\} \cup \{0\}\Big);$$

due to (3.40) we have $\operatorname{decay}(\boldsymbol{\gamma}) \geq 1$. For each weight $\gamma_j$ let $k_{\gamma_j}$ be the kernel from Lemma 3.6.1. With the help of the weights we can define spaces of functions of finitely many variables. For $d \in \mathbb{N}$ we define the reproducing kernel $K_d^{\boldsymbol{\gamma}}$ on $D^d \times D^d$ by

$$K_d^{\boldsymbol{\gamma}}(\mathbf{x},\mathbf{y}) := \prod_{j=1}^{d} (1 + k_{\gamma_j}(x_j, y_j)), \qquad \mathbf{x},\mathbf{y} \in D^d. \tag{3.41}$$

The reproducing kernel Hilbert space $H(K_d^{\boldsymbol{\gamma}})$ is the (Hilbert space) tensor product of the spaces $H(1 + k_{\gamma_j})$.

Now we want to define a space of functions of infinitely many variables. The natural domain for the counterpart of (3.41) for infinitely many variables is given by

$$\mathfrak{X}^{\boldsymbol{\gamma}} := \Big\{\mathbf{x} \in D^{\mathbb{N}} \,\Big|\, \prod_{j=1}^{\infty} (1 + k_{\gamma_j}(x_j, x_j)) < \infty\Big\}. \tag{3.42}$$

Let $a, a_1, \ldots, a_n \in D$ be arbitrary. Due to [42, Lemma 2.2] we have $(a_1, \ldots, a_n, a, a, \ldots) \in \mathfrak{X}^{\boldsymbol{\gamma}}$, and in particular $\mathfrak{X}^{\boldsymbol{\gamma}} \neq \emptyset$. We define the reproducing kernel $K_\infty^{\boldsymbol{\gamma}}$ on $\mathfrak{X}^{\boldsymbol{\gamma}} \times \mathfrak{X}^{\boldsymbol{\gamma}}$ by

$$K_\infty^{\boldsymbol{\gamma}}(\mathbf{x},\mathbf{y}) := \prod_{j=1}^{\infty} (1 + k_{\gamma_j}(x_j, y_j)), \qquad \mathbf{x},\mathbf{y} \in \mathfrak{X}^{\boldsymbol{\gamma}}. \tag{3.43}$$

For a function $f\colon D^d \to \mathbb{R}$ we define $\psi_d f\colon \mathfrak{X}^{\boldsymbol{\gamma}} \to \mathbb{R}$ by

$$(\psi_d f)(\mathbf{x}) = f(x_1, \ldots, x_d) \quad \text{for } \mathbf{x} \in \mathfrak{X}^{\boldsymbol{\gamma}}. \tag{3.44}$$

Due to [42, Lemma 2.3] $\psi_d$ is a linear isometry from $H(K_d^{\boldsymbol{\gamma}})$ into $H(K_\infty^{\boldsymbol{\gamma}})$, and

$$\bigcup_{d\in\mathbb{N}} \psi_d(H(K_d^{\boldsymbol{\gamma}})) \quad \text{is a dense subspace of } H(K_\infty^{\boldsymbol{\gamma}}). \tag{3.45}$$

### 3.6.2 The Integration Problem

To obtain a well-defined integration problem we assume that $\rho$ is a probability measure on (a $\sigma$-algebra on) $D$ such that

$$H \subseteq L^1(D, \rho).$$

Let $\rho^d$ denote the corresponding product measure on (the product $\sigma$-algebra on) $D^d$. Furthermore, we define the infinite product measure $\rho^{\mathbb{N}} = \otimes_{n\in\mathbb{N}}\rho$ on (the product $\sigma$-algebra on) $D^{\mathbb{N}}$, which again is a probability measure (see, e.g., [65, Sect. 14.3]).

Due to [42, Lemma 3.1] we have for all $d \in \mathbb{N}$ that

$$H(K_d^\gamma) \subseteq L^1(D^d, \rho^d),$$

and the respective embeddings $J_d$ from $H(K_d^\gamma)$ into $L^1(D^d, \rho^d)$ are continuous with

$$\sup_{d\in\mathbb{N}} \|J_d\|_{\mathrm{op}} < \infty. \tag{3.46}$$

Define the linear functional $I_d\colon H(K_d^\gamma) \to \mathbb{R}$ by

$$I_d(f) = \int_{D^d} f \,\mathrm{d}\rho^d, \qquad f \in H(K_d^\gamma).$$

Note that $\|I_d\|_{\mathrm{op}} \geq 1$, since $I_d(1) = 1$ and $\|1\|_{K_d^\gamma} = 1$. Furthermore, $\|I_d\|_{\mathrm{op}} \leq \|J_d\|_{\mathrm{op}}$, and therefore (3.46) implies

$$1 \leq \sup_{d\in\mathbb{N}} \|I_d\|_{\mathrm{op}} < \infty. \tag{3.47}$$

This yields the existence of a uniquely determined bounded linear functional

$$I_\infty\colon H(K_\infty^\gamma) \to \mathbb{R} \quad \text{such that} \quad I_\infty(\psi_d f) = I_d(f) \quad \text{for all } f \in H(K_d^\gamma), d \in \mathbb{N}, \tag{3.48}$$

cf. [42, Lemma 3.2].

Note that every $f \in H(K_\infty^\gamma)$ is measurable with respect to the trace of the product $\sigma$-algebra on $D^{\mathbb{N}}$. (This follows from (3.45), (3.46), and the fact that the pointwise limit of measurable functions is again measurable.)

If $\mathfrak{X}^\gamma$ is measurable, $\rho^{\mathbb{N}}(\mathfrak{X}^\gamma) = 1$, and $H(K_\infty^\gamma) \subseteq L^1(\mathfrak{X}^\gamma, \rho^{\mathbb{N}})$, then the bounded linear functional (3.48) is given by

$$I_\infty(f) = \int_{\mathfrak{X}^\gamma} f \,\mathrm{d}\rho^{\mathbb{N}} \quad \text{for all } f \in H(K_\infty^\gamma).$$

For sufficient conditions under which these assumptions are fulfilled we refer to [45].

We consider the integration problem on $H(K_\infty^\gamma)$ i.e. the approximation of the functional $I_\infty$ by randomized algorithms that use function evaluations (i.e., *standard information*) as admissable information.

### 3.6.3 The Unrestricted Subspace Sampling Model

We use the cost model introduced in [68], which we refer to as *unrestricted subspace sampling model*. It only accounts for the cost of function evaluations. To define the cost of a function evaluation, we fix an anchor $a \in D$ and a non-decreasing function

$$\$ : \mathbb{N}_0 \to [1, \infty].$$

Put

$$\mathcal{U} := \{u \subset \mathbb{N} \,|\, |u| < \infty\}.$$

For each $u \in \mathcal{U}$ put

$$\mathcal{T}_u := \{\mathbf{t} \in D^{\mathbb{N}} \,|\, t_j = a \text{ for all } j \in \mathbb{N} \setminus u\}.$$

To simplify the representation, we confine ourselves to non-adaptive randomized linear algorithms of the form

$$Q(f) = \sum_{i=1}^{n} w_i f(\boldsymbol{t}^{(i)}), \tag{3.49}$$

where the number $n \in \mathbb{N}$ of knots is fixed and the knots $\boldsymbol{t}^{(i)}$ as well as the coefficients $w_i \in \mathbb{R}$ are random variables with values in some $\mathcal{T}_{v_i}$, $v_i \in \mathcal{U}$, and in $\mathbb{R}$, respectively. (We discuss a larger class of algorithms in Remark 3.6.8.) The cost of $Q$ is given by

$$\mathrm{cost}(Q) = \sum_{i=1}^{n} \inf\{\$(|u|) \mid u \in \mathcal{U} \text{ such that } \boldsymbol{t}^{(i)}(\omega) \in \mathcal{T}_u \text{ for all } \omega \in \Omega\}. \tag{3.50}$$

In the definition of the cost function an inclusion property has to hold for all $\omega \in \Omega$. Often this worst case point of view is replaced by an average case (cf., e.g., [77] or [16, 40, 97]). We stress that such a replacement would not affect the cost of the algorithms that we employ to establish our upper bounds for the $N$-th minimal errors; for lower bounds cf. Remark 3.6.8(iii).

Let $\mathrm{x} \in \{\mathrm{d}, \mathrm{r}, \mathrm{w}\}$. For $N \geq 0$ let us define the *$N$-th minimal error on $H(K_\infty^\gamma)$* by

$$e^{\mathrm{x}}(N, K_\infty^\gamma) := \inf\{e^{\mathrm{x}}(I_\infty, Q) \,|\, Q \text{ as in (3.49) and } \mathrm{cost}(Q) \leq N\},$$

where in the case $\mathrm{x} = \mathrm{d}$ the algorithms have to be deterministic, while in the case $\mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}$ they are allowed to be randomized. The *(polynomial) convergence order of the $N$-th minimal errors of infinite-dimensional integration* is given by

$$\lambda^{\mathrm{x}}(K_\infty^\gamma) := \sup\Big\{\alpha \geq 0 \mid \sup_{N \in \mathbb{N}} e^{\mathrm{x}}(N, K_\infty^\gamma) \cdot N^\alpha < \infty\Big\}. \tag{3.51}$$

In analogy to our definitions for infinite-dimensional integration, we consider for univariate integration on $H(1 + k_1)$ also linear randomized algorithms $Q$ of the form (3.49), except that this time the knots $\boldsymbol{t}^{(i)}$ are, of course, random variables with values in $D$. The cost of such an algorithm is simply the number $n$ of function evaluations, and *$N$-th minimal errors on $H(1 + k_1)$* are given by

$$e^{\mathrm{x}}(N, 1 + k_1) := \inf\{e^{\mathrm{x}}(I_1, Q) \,|\, Q \text{ as in (3.49) and } n \leq N\}.$$

The *(polynomial) convergence order of the $N$-th minimal errors of univariate integration* is given by

$$\lambda^{\mathrm{x}}(1+k_1) := \sup\Big\{\alpha \geq 0 \mid \sup_{N\in\mathbb{N}} e^{\mathrm{x}}(N, 1+k_1)\cdot N^{\alpha} < \infty\Big\}.$$

**Remark 3.6.3.** Let $K \in \{K_\infty^\gamma, 1+k_1\}$ and, accordingly, $I \in \{I_\infty, I_1\}$. Obviously,

$$e^{\mathrm{r}}(N,K) \leq e^{\mathrm{w}}(N,K) \leq e^{\mathrm{d}}(N,K), \quad \text{and thus} \quad \lambda^{\mathrm{r}}(K) \geq \lambda^{\mathrm{w}}(K) \geq \lambda^{\mathrm{d}}(K).$$

Furthermore, it is easy to see that $e^{\mathrm{w}}(N,K) \geq e^{\mathrm{d}}(N,K)$ holds: If $Q$ is an arbitrary randomized algorithm of the form (3.49) with $\mathrm{cost}(Q) \leq N$, then for every $\omega \in \Omega$ the cost of the deterministic algorithm $Q(\omega)$ is at most $N$, implying

$$\sup_{\|f\|_K \leq 1} |(I - Q(\omega))f| \geq e^{\mathrm{d}}(N,K),$$

which in turn leads to $e^{\mathrm{w}}(I,Q) \geq e^{\mathrm{d}}(N,K)$. Hence we obtain

$$e^{\mathrm{w}}(N,K) = e^{\mathrm{d}}(N,K) \quad \text{and} \quad \lambda^{\mathrm{w}}(K) = \lambda^{\mathrm{d}}(K). \tag{3.52}$$

**Remark 3.6.4.** It is a well-known fact that for the reproducing kernel $K$ of the Korobov space $K_r([0,1))$ (see Example 3.6.2 ) we have $\lambda^{\mathrm{r}}(K) = r + \frac{1}{2}$. Details may be found e.g. in [111, Section 5]. Furthermore, one may check that $\lambda^{\mathrm{d}}(K) = r$, which, due to (3.52) implies that also $\lambda^{\mathrm{w}}(K) = r$.

### 3.6.4 A Sharp Result on Infinite-Dimensional Integration

The next theorem determines the exact polynomial convergence rate of the $N$-th minimal errors of infinte-dimensional integration on weighted reproducing kernel Hilbert spaces. We use the traditional Big-$O$-notation (Landau notation) and for two non-negative functions $f, g$, we write additionally $f = \Omega(g)$ if $g = O(f)$.

**Theorem 3.6.5.** *Let* $\mathrm{x} \in \{\mathrm{r}, \mathrm{w}\}$. *If the cost function* $\$$ *satisfies* $\$(\nu) = \Omega(\nu)$ *and* $\$(\nu) = O(e^{\sigma\nu})$ *for some* $\sigma \in (0,\infty)$, *then we have*

$$\lambda^{\mathrm{x}}(K_\infty^\gamma) = \min\left\{\lambda^{\mathrm{x}}(1+k_1), \frac{\mathrm{decay}(\boldsymbol{\gamma})-1}{2}\right\}. \tag{3.53}$$

Notice that the theorem implies that in the randomized setting infinite-dimensional integration on weighted reproducing kernel Hilbert spaces is (essentially) not harder than the corresponding univariate integration problem (as far as the polynomial convergence rate is concerned) as long as the weights decay fastly enough, i.e., as long as

$$\mathrm{decay}(\boldsymbol{\gamma}) \geq 2\lambda^{\mathrm{x}}(1+k_1) + 1.$$

*Proof.* Let us first consider the case x = r. In the special case where the reproducing kernel $k_1$ is *anchored in* $a$ (i.e., $k_1(a,a) = 0$) and satisfies $\gamma k_1 = k_\gamma$ for all $\gamma > 0$ (cf. Lemma 3.6.1), the statement of the Theorem follows from [40] and from [97] in combination with Theorem 3.5.4, as we will explain below in detail.

For a general reproducing kernel $k_1$ we need to find a suitably associated reproducing kernel $k_a$ anchored in $a$ and satisfying $\gamma k_a = (k_a)_\gamma$ for all $\gamma > 0$ to employ the embedding machinery from [42] to obtain the desired result (3.53). To this purpose we consider the bounded linear functional $\xi : H \to \mathbb{R}$, $f \mapsto f(a)$, where $a \in D$ is our fixed anchor. We define a new pair of seminorms on $H$ by

$$\|f\|_{1,a} := |\xi(f)| \quad \text{and} \quad \|f\|_{2,a} := \|f - \xi(f)\|_H.$$

Notice that $\|\cdot\|_{1,a}$ is induced by the symmetric bilinear form $\langle f, g\rangle_{1,a} := \xi(f) \cdot \xi(g)$. This new pair of seminorms satisfies obviously assumption (A2) and the norms $\|\cdot\|_H = (\|\cdot\|_1^2 + \|\cdot\|_2^2)^{1/2}$ and $\|\cdot\|_{H,a} := (\|\cdot\|_{1,a}^2 + \|\cdot\|_{2,a}^2)^{1/2}$ are equivalent norms on $H$. Hence $\|\cdot\|_{H,a}$ turns $H$ into a reproducing kernel Hilbert space, and satisfies (3.38) with $c = 1$ since

$$\|f\|_{H,a} \le \|f\|_{1,a} + \|f\|_{2,a} = |\langle f, 1\rangle_{1,a}| + \|f\|_{2,a} \quad \text{for all } f \in H.$$

Thus the new pair of seminorms satisfies also (A3). Furthermore, if $k_a$ is the reproducing kernel on $D \times D$ such that

$$H(k_a) = \{f \in H \mid f(a) = 0\}$$

and

$$\|f\|_{k_a} = \|f\|_{1+k_a} = \|f\|_{H,a} \quad \text{for all } f \in H(k_a),$$

then $k_a$ is anchored in $a$ and moreover we have $H(1 + k_a) = H$ as vector spaces, $H(1) \cap H(k_a) = \{0\}$, and

$$\|f\|_{1+\gamma k_a}^2 = \|f\|_{1,a}^2 + \frac{1}{\gamma}\|f\|_{2,a}^2$$

for all $\gamma > 0$, $f \in H$, implying $(k_a)_\gamma = \gamma k_a$, see [42, Rem. 2.2]. Since $\|\cdot\|_H = \|\cdot\|_{1+k_1}$ and $\|\cdot\|_{H,a} = \|\cdot\|_{1+k_a}$ are equivalent norms on $H(1 + k_1) = H = H(1 + k_a)$, we obtain $\lambda^{\mathrm{r}}(1 + k_1) = \lambda^{\mathrm{r}}(1 + k_a)$. Due to [42, Thm. 2.3] we have

$$\mathfrak{X}^{\gamma,a} := \Big\{\mathbf{x} \in D^{\mathbb{N}} \,\Big|\, \prod_{j=1}^{\infty}(1 + \gamma_j k_a(x_j, x_j)) < \infty\Big\} = \mathfrak{X}^{\gamma}.$$

According to (3.43) we define $K_\infty^{\gamma,a} : \mathfrak{X}^\gamma \times \mathfrak{X}^\gamma \to \mathbb{R}$ by

$$K_\infty^{\gamma,a}(\mathbf{x}, \mathbf{y}) := \prod_{j=1}^{\infty}(1 + \gamma_j k_a(x_j, y_j)) \quad \text{for } \mathbf{x}, \mathbf{y} \in \mathfrak{X}^\gamma.$$

Now we consider the integration problem in $H(K_\infty^{\gamma,a})$ and may use [40, Subsect. 3.2.1] and [97, Cor. 1] in combination with Theorem 3.5.4. Indeed, due to Theorem 3.5.4 we

may choose linear randomized algorithms with convergence rates $\alpha$ arbitrarily close to $\lambda^{\mathrm{r}}(1+k_1) = \lambda^{\mathrm{r}}(1+k_a)$ to obtain via the randomized Smolyak method algorithms that satisfy (3.27) for $\mathrm{x} = \mathrm{r}$ (and consequently also [97, Eqn. (10)]). Now [97, Cor. 1] ensures that

$$\lambda^{\mathrm{r}}(K_\infty^{\boldsymbol{\gamma},a}) \geq \min\left\{\lambda^{\mathrm{r}}(1+k_1),\, \frac{\mathrm{decay}(\boldsymbol{\gamma})-1}{2}\right\}.$$

Furthermore, we have due to [40, Eqn. (21)]

$$\lambda^{\mathrm{r}}(K_\infty^{\boldsymbol{\gamma},a}) \leq \min\left\{\lambda^{\mathrm{r}}(1+k_1),\, \frac{\mathrm{decay}(\boldsymbol{\gamma})-1}{2}\right\}.$$

Due to [42, Cor. 5.1] these estimates also hold for $H(K_\infty^{\boldsymbol{\gamma}})$.

Let us now consider the case $\mathrm{x} = \mathrm{w}$. Due to (3.52), identity (3.53) follows directly from the deterministic result [42, Theorem 5.1]. □

We now provide two corollaries and add some remarks.

Theorem 3.6.5, which deals with randomized algorithms, and the corresponding deterministic theorem [42, Theorem 5.1] allow immediately to compare the power of deterministic and randomized algorithms.

**Corollary 3.6.6.** *Let the assumptions of Theorem 3.6.5 hold. For infinite-dimensional integration on $H(K_\infty^{\boldsymbol{\gamma}})$ randomized algorithms are superior to deterministic algorithms, i.e., $\lambda^{\mathrm{r}}(K_\infty^{\boldsymbol{\gamma}}) > \lambda^{\mathrm{d}}(K_\infty^{\boldsymbol{\gamma}})$, if and only if*

$$\lambda^{\mathrm{r}}(1+k_1) > \lambda^{\mathrm{d}}(1+k_1) \quad \textit{and} \quad \mathrm{decay}(\boldsymbol{\gamma}) > 1 + 2\lambda^{\mathrm{d}}(1+k_1)$$

*are satisfied.*

The next corollary on infinite-dimensional integration on weighted Korobov spaces in the randomized setting parallels [42, Theorem 5.5], which discusses the deterministic setting.

**Corollary 3.6.7.** *Let $r > 1/2$, and let the univariate reproducing kernel $k_1$ be as in (3.39). Then the weighted Korobov space $H(K_\infty^{\boldsymbol{\gamma}})$ is an infinite tensor product of the periodic Korobov space $H(1+k_1) = K_r([0,1))$ of smoothness $r$, see Example 3.6.2. If the cost function $\$$ satisfies $\$(\nu) = \Omega(\nu)$ and $\$(\nu) = O(e^{\sigma\nu})$ for some $\sigma \in (0,\infty)$, then we have*

$$\lambda^{\mathrm{r}}(K_\infty^{\boldsymbol{\gamma}}) = \min\left\{r+\frac{1}{2},\, \frac{\mathrm{decay}(\boldsymbol{\gamma})-1}{2}\right\} \quad \textit{and} \quad \lambda^{\mathrm{w}}(K_\infty^{\boldsymbol{\gamma}}) = \min\left\{r,\, \frac{\mathrm{decay}(\boldsymbol{\gamma})-1}{2}\right\}.$$

*Proof.* Since $\lambda^{\mathrm{r}}(1+k_1) = r+1/2$ and $\lambda^{\mathrm{w}}(1+k_1) = r$ (see Remark 3.6.4), Theorem 3.6.5 immediately yields the result for $\lambda^{\mathrm{r}}(K_\infty^{\boldsymbol{\gamma}})$ and $\lambda^{\mathrm{w}}(K_\infty^{\boldsymbol{\gamma}})$.

Notice that the result for $\lambda^{\mathrm{w}}(K_\infty^{\boldsymbol{\gamma}})$ can also be derived from Remark 3.6.3 and [42, Theorem 5.5]. □

**Remark 3.6.8.** Let us come back to Theorem 3.6.5.

(i) Algorithms that achieve convergence rates arbitrarily close to $\lambda^{\mathrm{x}}(K_\infty^\gamma)$ are, e.g., *multivariate decomposition methods (MDMs)* that were introduced in [68] (in the deterministic setting) and developed further in [97] (in the deterministic and in the randomized setting); originally, these algorithms were called *changing dimension algorithms*, cf., e.g., [15, 16, 40, 68, 97]. MDMs exploit that the anchored function decomposition of an integrand can be efficiently computed; a method for multivariate integration based on the same idea is the *dimension-wise integration method* proposed in [50]. To achieve (nearly) optimal convergence rates, the MDMs may employ as building blocks Smolyak algorithms for multivariate integration that rely on (nearly) optimal algorithms for univariate integration on $H(1+k_1)$, cf. [97, Section 3.3] and the proof of Theorem 3.6.5.

(ii) In the special case where $\mathrm{x} = \mathrm{r}$ and where $k_1$ is an *ANOVA-kernel* (i.e., $k_1$ satisfies $\int_D k_1(y,x)\,\mathrm{d}x = 0$ for every $y \in D$) a version of Theorem 3.6.5 was already proved in [16, Theorem 4.3]. It was the first result that rigorously showed that MDMs can achieve the optimal order of convergence also on spaces with norms that are *not* induced by an underlying anchored function space decomposition. It was not derived with the help of function space embeddings, but by an elaborate direct analysis. Apart from addressing only the ANOVA setting, a further drawback of [16, Theorem 4.3] is that its assumptions are slightly stronger than the ones made in Theorem 3.6.5: It is not sufficient to know the convergence rate of the $N$-th minimal errors of the univariate integration problem, but additionally one has to verify the existence of unbiased randomized algorithms for multivariate integration that satisfy certain variance bounds, see [16, Assumption 4.1]. Nevertheless, in many important cases it is well known that such variance bounds hold. Furthermore, one should mention that the analysis in [16] ist not restricted to product weights as in this section, but is done for general weights.

Note that the kernel $k_1$ of the Korobov space $K_r([0,1))$ from Example 3.6.2 and Corollary 3.6.7 is actually an ANOVA kernel. Hence the identity for $\lambda^{\mathrm{r}}(K_\infty^\gamma)$ in Corollary 3.6.7 may also be derived by employing [16, Theorem 4.3] after verifying the existence of unbiased algorithms for multivariate integration that satisfy [16, Assumption 4.1].

(iii) The upper bound for $\lambda^{\mathrm{r}}(K_\infty^\gamma)$ in (3.53) relies on the corresponding bound [40, Eqn. (21)] for the case where the univariate reproducing kernel $k_1$ is anchored in $a$. Although the definition of the cost function in [40] takes the average case and not the worst case point of view and differs therefore from (3.50), both definitions lead to the same cost for the admissable class of algorithms $\mathcal{A}^{\mathrm{res}}$ considered in the unrestricted subspace sampling model in [40]. The class $\mathcal{A}^{\mathrm{res}}$ contains not only algorithms of the form (3.49), but also adaptive and non-linear algorithms. In the proof of Theorem 3.6.5 we employ the function space embeddings from [42], which allows us to transfer results for linear algorithms from the case of anchored kernels to the general case. Hence we can conclude that the upper bound for $\lambda^{\mathrm{r}}(K_\infty^\gamma)$ in (3.53)

holds also if we admit adaptive linear algorithms of the form (3.49) for infinite-dimensional as well as for univariate integration, but we do not know whether this is still the case if we admit non-linear algorithms.

We finish this section with some remarks on extensions of our results on infinte-dimensional integration to other settings.

**Remark 3.6.9.** To obtain computational tractability of problems depending on a high or infinite number of variables, it is usually essential to be able to arrange the variables in such a way that their impact decays sufficiently fast. One approach to model the decreasing impact of successive variables is to use weighted function spaces, like the ones we defined and studied in this section, to moderate the influence of groups of variables. This approach goes back to the seminal paper [103]. Another approach is the concept of *increasing smoothness* with respect to properly ordered variables, see, e.g., [24, 43, 51, 63, 66, 92, 102]. The precise definition of Hilbert spaces of functions depending on infinitely many variables of increasing smoothness can be found in [43, Section 3]. Now [43, Theorem 3.19] shows how to relate these spaces to suitable weighted Hilbert spaces via mutual embeddings, making it therefore easy to transfer our results in the randomized setting, Theorem 3.6.5 and Corollary 3.6.7, from weighted spaces to spaces with increasing smoothness, cf. [43, Theorem 4.5 and Corollary 4.7] for the corresponding transference results in the deterministic setting.

Instead of applying Theorem 3.5.4 to the infinite-dimensional integration problem, we may also use it to tackle the *infinite-dimensional $L_2$-approximation problem*. Indeed, a sharp result for the latter problem was obtained in [115, Corollary 9] in the deterministic setting for weighted anchored reproducing kernel Hilbert spaces with the help of multivariate decomposition methods based on Smolyak algorithms (cf. [118, Theorem 7]). The analysis relies on explicit cost bounds for deterministic Smolyak algorithms from [116]. In [43, Theorem 4.5] the result is extended to weighted (not necessarily anchored) reproducing kernel Hilbert spaces (relying on the embedding tools from [42]) and to spaces of increasing smoothness.

Now one may use Theorem 3.5.4 to establish a corresponding result to [115, Corollary 9] for weighted anchored spaces in the randomized setting and may generalize it to non-anchored weighted spaces and to spaces of increasing smoothness via the embedding results established in [42, 43].

To work out all the details of these generalizations is beyond the scope of this dissertation.

# Chapter 4

# Randomized Smolyak Method for Integration on Haar-Wavelet Spaces

## 4.1 Introduction

In this chapter we consider the integration problem over the domain $[0,1)^D$, where $D = d \cdot s$ for some $d, s \in \mathbb{N}$. The spaces of integrands are certain Haar-wavelet spaces, consisting of square integrable functions whose Haar-wavelet coefficients decay fastly enough. We analyze the performance of randomized Smolyak algorithms that use as building blocks scrambled $(0, m, s)$-nets in some base $b$. The considered error criterion is the randomized error. We pursue mainly two aims:

Firstly, we want to show that under more specific assumptions on the approximation problem (compared with Chapter 3) we may improve on the general upper error bounds for randomized Smolyak algorithms. (This phenomenon is also known for deterministic Smolyak algorithms, see, e.g., [116, 44, 85].) "More specific" means here that we consider an integration problem (instead of a general linear approximation problem) and a specific reproducing kernel Hilbert space defined via the decay of Haar-wavelet coefficients (instead of a general tensor product Hilbert space of functions) as input space. We are able to show via a lower error bound (see Theorem 4.2.16) that our upper improved error bound provided in Theorem 4.2.11 is sharp, i.e., that our Smolyak algorithms based on scrambled nets cannot achieve a higher rate of convergence. This means we have determined the exact asymptotic convergence rate of the randomized error of our algorithms.

Secondly, we want to make a precise comparison between randomized quasi-Monte Carlo (RQMC) algorithms based on scrambled $(0, m, s)$-nets (that can be seen as specialized algorithms, tuned for the specific integration problem) on the one hand and Smolyak algorithms based on one-dimensional nets (which can be seen as special instances of a universal method) on the other hand.

This comparison is motivated by the comparison done in [19]. In [19] Dick et al. investigate a specific instance of the randomized Smolyak method for the integration problem in certain Sobolev spaces over $[0,1)^D$, $D = d \cdot s$. Firstly, they consider higher-order digital sequences in $[0,1)^s$ with a fixed digital shift and use them as building blocks

for their $D$-dimensional Smolyak construction. They prove that the resulting integration algorithms achieve almost optimal order of convergence (up to logarithmic factors) of the worst-case error. Secondly, they randomize their construction by chosing the digital shift randomly and achieve for the resulting randomized Smolyak construction a corresponding convergence order of the root mean square worst-case error (which is obtained by averaging the square of the worst-case error over all digital shifts and then taking the square root). The authors studied Smolyak algorithms for all possible combinations of $d$ and $s$ with $d \cdot s = D$, starting with $s = 1, d = D$, i.e., Smolyak algorithms based on one-dimensional nets, up to $s = D, d = 1$, i.e., pure higher-order nets in dimension $D$. Their error bounds get larger for larger $d$ by essentially a factor of $(\log N)^{d \cdot \alpha}$, where $N$ is the number of sample points employed by the Smolyak method and $\alpha$ is the degree of smoothness of the considered Sobolev space, see [19, Corollary 4.2]. Since Dick et al. did not provide matching lower bounds (and we actually believe that their upper bounds are not optimal with respect to the logarithmic order), the question remains whether this really gives a faithful picture of the changes in the convergence order of the error. Moreover, the error criterion used in [19], the root mean square worst-case error, is a rather untypical error criterion for randomized algorithms.

That is why we perform a comparison of Smolyak algorithms based on scrambled $(0, m, s)$-nets for all possible combinations of $d$ and $s$ with $d \cdot s = D$ in the Haar-wavelet space setting with respect to the commonly used randomized error criterion. Due to Heinrich et al. [55] the exact convergence order of scrambled $(0, m, s)$-nets is known, and our results determine the exact convergence order of Smolyak algorithms based on scrambled nets. Therefore we can deduce that the convergence order of the randomized error decreases for increasing $d$ by a factor $(\log N)^{(d-1)(1+\alpha)}$, where again $N$ is the number of sample points employed by the algorithm at hand and $\alpha$ is the "degree of smoothness" of the considered Haar wavelet space. This factor describes the loss in the convergence order we have to accept in this setting if we use for integration a universal tool (Smolyak's method) instead of the more specialized, optimal tool, namely scrambled $(0, m, D)$-nets.

## 4.2 Multivariate Integration on Haar-Wavelet Spaces: Smolyak vs. $(0, m, s)$-Nets

We are considering the problem of integrating $D-$variate functions belonging to Haar-wavelet spaces with smoothness parameter $\alpha > \frac{1}{2}$. The solution operator is the integration operator $I_D$, which is given by

$$I_D : \mathcal{H}_\alpha^D \to \mathbb{R}, \quad I_D f = \int_{[0,1)^D} f(\mathbf{x})\, d\,\mathbf{x}\,.$$

The $D-$variate Haar-wavelet space $\mathcal{H}_\alpha^D$ with smoothness parameter $\alpha$ consists of all square-integrable functions whose wavelet coefficients converge to 0 quickly enough, see Definition 4.2.4. We would like to use the randomized Smolyak method with building blocks being scrambled $(0, m, s)-$nets, where $D = ds$ for some $d \in \mathbb{N}$. The building blocks

$((U_l^{(n)})_{l\in\mathbb{N}})_{n\in[d]}$ of our Smolyak method are randomized QMC quadratures such that for every $n = 1, \dots, d, l \in \mathbb{N}$, quadrature $\mathrm{U}_l^{(n)}$ is based on a scrambled $(0, l-1, s)$-net in base $b$, i.e. for some scrambled $(0, l-1, s)-$net $(Y_i)_{i=1}^{b^{l-1}}$ and any function $f$ it holds

$$U_l^{(n)} f = b^{-l+1} \sum_{i=1}^{b^{l-1}} f(Y_i).$$

For the definition of scrambled $(0, m, s)-$nets in base $b$ see Section 4.2.1. We make the standing assumption that all the building blocks $U_l^{(n)}, n = 1, \dots, d, l \in \mathbb{N}$, are randomized independently.

Recall the construction of the randomized $d-$variate Smolyak method of level $L$, see Definition 3.3.1. Our focus lies on the *randomized error* $e^{\mathrm{r}}(I_D, A(L,d))$ of the Smolyak method, which is given by

$$e^{\mathrm{r}}(I_D, A(L,d)) = \sup_{\|f\|_{\mathcal{H}_\alpha^D}\leq 1} \left(\mathbf{E}\left[|A(L,d)f - I_D f|^2\right]\right)^{\frac{1}{2}}.$$

We denote by $N = N(L,d)$ the number of function evaluations performed by the Smolyak method $A(L,d)$. Our aim is to show that there exist constants $c, C > 0$ independent of $N$ such that

$$c\frac{(\log(N))^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}} \leq e^{\mathrm{r}}(I_D, A(L,d)) \leq C\frac{(\log(N))^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}.$$

Compared with Theorem 3.5.4 and Corollary 3.5.12 this gives the exact order of convergence of randomized error (note however, that the bounds from Chapter 3 are much more general since they can be applied to any linear approximation problem in a Hilbert space setting). Changing the parameter $d$ from 1 to $D$ through the divisors of $D$ yields a whole family of algorithms, from quadratures based purely on $(0, m, D)$-nets to Smolyak methods with building blocks stemming from one-dimensional nets.

**Remark 4.2.1.** Let $L \geq d$. Notice that since the weights of the building block quadratures $U_l^{(n)}$ sum up to 1, the same holds true for $A(L,d)$, i.e.,

$$A(L,d)f = \sum_{\nu=1}^{N} w_\nu f(x_\nu) \tag{4.1}$$

with suitable $w_\nu \in \mathbb{R}$, and deterministic or random points $x_\nu \in [0,1)^D$, where $\sum_{\nu=1}^N w_\nu = 1$. Indeed, for arbitrary quadratures $Q^{(1)}, \dots, Q^{(d)}$, such that

$$Q^{(n)} f = \sum_{j=1}^{N_n} w_j^{(n)} f(x_j^{(n)}), \quad n = 1, \dots, d,$$

denoting $w^{(n)} := \sum_{j=1}^{N_n} w_j^{(n)}$, we have that the sum of the weights used by the quadrature $Q := \bigotimes_{n=1}^d Q^{(n)}$ is equal to $\prod_{n=1}^d w^{(n)}$. Now, the sum of the weights used by $\Delta_{l_n}^{(n)}$ is equal

to 0 if $l_n > 1$ and is equal to 1 if $l_n = 1$. It follows that the sum of weights used by $A(L,d)$ is equal to the sum of weights used by $\bigotimes_{n=1}^{d} \Delta_1^{(n)}$, i.e. to 1.

One may easily find examples where weights applied by our construction are negative, so in particular $A(L,d)$ is not a (randomized) QMC quadrature.

Note in passing that utilizing representation (3.4) one may also find an alternative formula for the sum of weights of our Smolyak algorithm, namely

$$\sum_{\nu=0}^{\min\{d-1,L-d\}} (-1)^{\nu} \binom{d-1}{\nu} \binom{L-\nu-1}{d-1}.$$

It follows that the above sum is equal to 1.

A few remarks on notation. If not explicitly stated otherwise all additions and substractions involving vectors and real numbers are performed coordinatewise, so e.g. for $\mathbf{k} = (k_1, \ldots, k_d) \in \mathbb{N}^d, \mathbf{j} = (j_1, \ldots, j_d) \in \mathbb{N}^d$ the formula $\mathbf{k} = \mathbf{j} - 1$ is to be read as $k_n = j_n - 1, n = 1, \ldots, d$.

In the sequel $b \in \mathbb{N}_{\geq 2}$ stands for the base of the net and is fixed. For $j \in \mathbb{N}_0$ put $\theta_j = \{0\}$ if $j = 0$ and $\theta_j = \{0, \ldots, b-1\}$ else. For $\mathbf{j} \in \mathbb{N}_0^t$ set

$$\theta_{\mathbf{j}} = \theta_{j_1} \times \cdots \times \theta_{j_t}.$$

Similarly put $\vartheta_j = \{0\}$ for $j \in \{-1, 0\}$ and $\vartheta_j = \{0, \ldots, b^j - 1\}$ for $j \in \mathbb{N}$. For $\mathbf{j} \in \mathbb{Z}_{\geq -1}^t$ set

$$\vartheta_{\mathbf{j}} = \vartheta_{j_1} \times \cdots \times \vartheta_{j_t}.$$

Finally, for a vector $\mathbf{v} = (v_1, \ldots, v_t)$ we write $|\mathbf{v}| := \sum_{j=1}^{t} |v_j|$.

### 4.2.1 Scrambled $(0, m, s)-$Nets

Fix $b \in \mathbb{N}_{\geq 2}$.

**Definition 4.2.2.** For $j \in \mathbb{N}_0$ and $k \in \vartheta_j$ we define the one-dimensional *elementary interval* $E_k^j$ to be

$$E_k^j := [kb^{-j}, (k+1)b^{-j}).$$

Moreover, we put

$$E_k^{-1} = [0, 1).$$

Let $s \in \mathbb{N}$. An $s-$dimensional interval is called *elementary* if for some $\mathbf{j} \in \mathbb{Z}_{\geq -1}^s$ and $\mathbf{k} \in \vartheta_{\mathbf{j}}$ it is of the form

$$E_{\mathbf{k}}^{\mathbf{j}} := E_{k_1}^{j_1} \times \cdots \times E_{k_s}^{j_s}.$$

**Definition 4.2.3.** Let $m, s \in \mathbb{N}$. A finite set $\mathcal{P} \subset [0,1)^s$ is called a $(0, m, s)-$*net* in base $b$ if each elementary $s-$dimensional interval of volume $b^{-m}$ contains exactly one point of $\mathcal{P}$.

The notion of $(0, m, s)-$nets was introduced by Niederreiter in [78]. Nets may be build using e.g. the Faure construction [26], [27].

The most common way of obtaining randomized nets is via scramblings, which was introduced by Owen, see e.g. [90],[91]. Here we present a slight modification of the original idea, see [75, Section 2.4.]. Generally speaking, a bijective mapping $\sigma : [0,1)^d \to [0,1)^d$ is called a ($b$-ary) scrambling of depth $l$ if for every elementary interval $E$ in base $b$ with $\lambda^d(E) \geq b^{-l}$ it holds that $\sigma(E)$ is an elementary interval and $\lambda^d(E) = \lambda^d(\sigma(E))$.

Here we are interested not in scramblings as mappings, but in an image of a $(0, m, s)$-net in base $b$ under a random $b$-ary scrambling of depth $l \geq m$. For that we use the following construction. A mapping $\sigma : [0,1) \to [0,1)$ is called a *discrete $b-$ary scrambling (of depth $l$)* if it is constructed in the following way. Let $x =_b 0.x_1x_2 \dots x_m x_{m+1} \dots$ be a $b-$ary representation of $x$ (whenever possible we choose the representation having finitely many digits different from 0). To determine $\sigma(x)$ we first fix some permutation $\pi$ of $\{0, 1, \dots, b-1\}$ and let the first $b-$ary digit of $\sigma(x)$ be $y_1 = \pi(x_1)$. Next for every possible value of $x_1$ we fix a permutation $\pi_{x_1}$ of $\{0, 1, \dots, b-1\}$ and define the second $b-$ary digit of $\sigma(x)$ to be $y_2 = \pi_{x_1}(x_2)$. Continuing analogously, for every $x_1, x_2$ we choose a permutation $\pi_{x_1,x_2}$ and let the third digit of $\sigma(x)$ be $y_3 = \pi_{x_1,x_2}(x_3)$. In this way, choosing permutations $\pi, \pi_{x_1}, \dots, \pi_{x_1,\dots,x_{l-1}}$ uniformly and independently, we get the first $l$ digits of $\sigma(x)$. There are many approaches concerning how to choose the remainder term. We fix all the other digits of $\sigma(x)$ to be equal 0. Proceeding this way, choosing all the permutations independently at random from the uniform distribution we obtain a discrete random $b$-ary scrambling. Let now $\mathcal{P} \subset [0,1)^s$ be a $(0, m, s)-$ net in base $b$ and let $\boldsymbol{\sigma} := (\sigma_1, \dots, \sigma_s)$ be a vector of independent discrete random scramblings of depth $l \geq m$. We define the set

$$\boldsymbol{\sigma}(\mathcal{P}) := \{(\sigma_1(p_{i,1}) + b^{-l}\xi_i^1, \dots, \sigma_s(p_{i,s}) + b^{-l}\xi_i^s) \,|\, (p_{i,1}, \dots, p_{i,s}) =: p_i \in \mathcal{P}\},$$

where the family of remainder terms $(\xi_i^t), i \in \mathbb{N}, t \in [s]$, consists of iid random variables distributed according to Unif([0,1)) and independent of all the permutations. If $\mathcal{P}$ is a $(0, m, s)-$net the same holds true for $\boldsymbol{\sigma}(\mathcal{P})$. Moreover, every single $p \in \boldsymbol{\sigma}(\mathcal{P})$ is distributed according to Unif($[0,1)^s$). We call the set $\boldsymbol{\sigma}(\mathcal{P})$ a *scrambled net.*

For every $l \in \mathbb{N}$ let $\boldsymbol{\sigma}_l^{(n)} := (\sigma_{l,t}^{(n)})_{t\in[s]}$ be a vector of independent discrete scramblings of depth $l-1$. We require all the permutations used by $((\sigma_{l,t}^{(n)})_{t\in[s]})_{n\in[d],l\in\mathbb{N}}$ and all the remainder terms $((\xi_{l,i}^{(n),t})_{t\in[s],i\in[b^{j-1}]})_{n\in[d],l\in\mathbb{N}}$ to be independent. We let $U_l^{(n)}$ be a QMC quadrature based on $\boldsymbol{\sigma}_l^{(n)}(\mathcal{P}_l^{(n)})$ for some $(0, l-1, s)$-net $\mathcal{P}_l^{(n)}$. We say in this case that all the building blocks $U_l^{(n)}, n = 1, \dots, d, l \in \mathbb{N}$, are scrambled independently.

Note that in the literature what we call a discrete scrambling with arbitrarily chosen remainder term is often referred to just as scrambling.

### 4.2.2 Function Spaces

Now we define Haar-wavelet spaces $\mathcal{H}_\alpha^D$. We start with univariate wavelets. Let $b \in \mathbb{N}_{\geq 2}$ be as in Section 4.2.1 (it will later coincide with the base of a $(0, m, s)-$net) and define

$$\psi_i(x) = b^{\frac{1}{2}}\,\mathbf{1}_{\lfloor bx\rfloor=i} - b^{-\frac{1}{2}}\,\mathbf{1}_{\lfloor x\rfloor=0}, \quad i = 0, 1, \dots, b-1,$$

here $\lfloor x \rfloor$ denotes the largest integer smaller or equal then $x$ and $\mathbf{1}_A$ is the characteristic function of the set $A$. For integers $j > 0$ and $k \in \vartheta_{j-1}$ put

$$\psi_{i,k}^j(x) := b^{\frac{j-1}{2}} \psi_i(b^{j-1}x - k) = b^{\frac{j-2}{2}} [b\, \mathbf{1}_{\lfloor b^j x \rfloor = bk+i} - \mathbf{1}_{\lfloor b^{j-1} x \rfloor = k}].$$

Note that $\psi_i = \psi_{i,0}^1$. Moreover, define

$$\psi_{0,0}^0 := \mathbf{1}_{[0,1)}\,.$$

We shall refer to those functions as *Haar wavelets*. The parameters have the following interpretation: $j$ describes the resolution of the wavelet, which corresponds to the size of its support, $i$ describes the shape and $k$ is the shift parameter. These wavelets are normalized with respect to the $L^2$-norm, i.e. $\|\psi_{i,k}^j\|_{L^2} = 1$. If $j > 0$ then we have $\operatorname{supp}(\psi_{i,k}^j) = E_k^{j-1}$, see Definition 4.2.2. For an integer $j \geq 0$ let us put

$$V_j := \{f \in L^2([0,1)) \,|\, f \text{ is constant on intervals } E_k^j, k \in \vartheta_j\}.$$

Moreover, we define $W_0 = V_0$ and $W_{j+1}$ to be the orthogonal complement of $V_j$ in $V_{j+1}$, i.e. we have

$$V_{j+1} = V_j \oplus W_{j+1} = \bigoplus_{\nu=0}^{j+1} W_\nu.$$

One may easily see that

$$W_j = \operatorname{span}\{\psi_{i,k}^j \,|\, i \in \theta_j; k \in \vartheta_{j-1}\}$$

and $\bigoplus_{j=0}^{\infty} W_j$ is dense in $L^2([0,1))$.

Now we proceed to multivariate wavelets which are nothing more then tensor products of univariate wavelets. Fix a dimension $D \in \mathbb{N}$ and let

$$J(D,L) := \left\{\mathbf{j} \in \mathbb{N}_0^D \,|\, |\,\mathbf{j}\,| = L\right\}.$$

We define the approximation space of level $L$ to be

$$V^{D,L} := \sum_{\mathbf{j} \in J(D,L)} \bigotimes_{t=1}^{D} V_{j_t}.$$

Moreover, let

$$W^{D,L} := \bigoplus_{\mathbf{j} \in J(D,L)} \bigotimes_{t=1}^{D} W_{j_t}.$$

Note that the space $W^{D,L}$ is represented as an orthogonal sum whereas $V^{D,L}$ is not. It is easily verified that $V^{D,L+1} = V^{D,L} \oplus W^{D,L+1}$.

Given vectors $\mathbf{j} \in \mathbb{N}_0^D, \mathbf{i} \in \theta_{\mathbf{j}}, \mathbf{k} \in \vartheta_{\mathbf{j}-1}$ we write

$$\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}(\mathbf{x}) := \prod_{t=1}^{D} \psi_{i_t,k_t}^{j_t}(x_t), \quad \mathbf{x} = (x_1, \ldots, x_D) \in [0,1)^D.$$

For notational reasons for a vector $\mathbf{v}$ we introduce

$$u(\mathbf{v}) := \{t \,|\, v_t \neq 0\}.$$

Note that the wavelets $(\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})_{\mathbf{j},\mathbf{i},\mathbf{k}}$ are not orthogonal but they do integrate to 0 as long as $u(\mathbf{j}) \neq \emptyset$. We may represent every function $f \in L^2([0,1)^D)$ as

$$f = \sum_{\mathbf{j},\mathbf{k},\mathbf{i}} \hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}} \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} := \sum_{\mathbf{j}} \sum_{\mathbf{k}} \sum_{\mathbf{i}} \hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}} \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} \tag{4.2}$$

with Haar coefficients

$$\hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}} = \int_{[0,1)^D} f(\mathbf{x}) \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}(\mathbf{x})\, d\,\mathbf{x}$$

(for details, see [91]). Functions $(\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})_{\mathbf{j},\mathbf{k},\mathbf{i}}$ form a tight frame in $L^2([0,1)^D)$, meaning that there exists a constant $c$ such that for every $f \in L^2([0,1)^D)$ it holds $\sum\limits_{\mathbf{j},\mathbf{i},\mathbf{k}} |\langle f, \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} \rangle_{L^2}|^2 = c\|f\|_{L^2}^2$ (in this special case we even have $c = 1$).

**Definition 4.2.4.** Let $\alpha > \frac{1}{2}, D \in \mathbb{N}$. The $D$-variate *Haar-wavelet space with smoothness* $\alpha$, denoted $\mathcal{H}_\alpha^D$, is given by

$$\mathcal{H}_\alpha^D := \left\{ f \in L^2([0,1)^D) \,\middle|\, \sum_{\mathbf{j},\mathbf{k},\mathbf{i}} b^{2\alpha|\mathbf{j}|} (\hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}})^2 < \infty \right\}.$$

We equip $\mathcal{H}_\alpha^D$ with the inner product

$$\langle f, g \rangle_{\mathcal{H}_\alpha^D} := \sum_{\mathbf{j},\mathbf{k},\mathbf{i}} b^{2\alpha|\mathbf{j}|} \hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}} \hat{g}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}}.$$

Scaled wavelets and scaled coefficients are denoted by $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j},\alpha} := b^{-\alpha|\mathbf{j}|} \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$ and $\hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j},\alpha} := b^{\alpha|\mathbf{j}|} \hat{f}_{\mathbf{i},\mathbf{k}}^{\mathbf{j}}$. Note that the scaled wavelets are normalized with respect to the $\mathcal{H}_\alpha^D$-norm. We want to represent a function $f \in \mathcal{H}_\alpha^D$ as a vector of wavelet coefficients. For $n \in \mathbb{N}_0$ put

$$J(n) := \{(\mathbf{j},\mathbf{k},\mathbf{i}) \in \mathbb{N}_0^D \times \mathbb{N}_0^D \times \mathbb{N}_0^D \,|\, |\,\mathbf{j}\,| = n, \mathbf{k} \in \vartheta_{\mathbf{j}-1}, \mathbf{i} \in \theta_{\mathbf{j}}\}.$$

Let $\hat{f}^n$ be a vector consisting of the wavelet coefficients of $f$ pertaining to indices from $J(n)$ ordered in some fixed way. Put

$$\hat{f} := (\hat{f}^n)_{n \in \mathbb{N}_0}^T.$$

In a similar fashion we define $\hat{f^\alpha}$. Ordering the functions $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$ in exactly the same way we obtain vectors of functions $\Psi$ and $\Psi^\alpha$. Using the above notation we may write identity (4.2) as

$$f = (\hat{f^\alpha})^T \Psi^\alpha.$$

Here $\mathbf{v}^T$ is just the transposed vector $\mathbf{v}$.

### 4.2.3 Upper Bounds on the Integration Error

We want to investigate the problem of integrating $D = sd$-variate functions from the Haar-wavelet space $\mathcal{H}_\alpha^D$. To this end we put

$$I_s : \mathcal{H}_\alpha^s \to \mathbb{R}, \quad I_s f = \int_{[0,1)^s} f(\mathbf{x})\, d\,\mathbf{x}\,.$$

Furthermore, $A(L,d)$ is the Smolyak method constructed as in Definition 3.3.1, where for $n = 1, \ldots, d, l \in \mathbb{N}$, $\mathrm{U}_l^{(n)}$ is a RQMC quadrature based on a scrambled $(0, l-1, s)$-net and all the building blocks are randomized independently.

We call the sets

$$B_a = \{as+1, as+2, \ldots (a+1)s\}, a = 0, 1 \ldots, d-1,$$

*blocks*. Given $\mathbf{j} \in \mathbb{N}_0^D$ we say that the block $B_a$ is *active (with respect to* $\mathbf{j}$*)* if

$$B_a \cap u(\mathbf{j}) \neq \emptyset.$$

With the obvious notation we have

$$\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} := \prod_{n=1}^{d} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}.$$

Note that $\mathrm{supp}(\Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}) = E_{\mathbf{k}_n}^{\mathbf{j}_n\,-1} \subseteq [0,1)^s$.

**Lemma 4.2.5.** *Consider* $\mathbf{j}, \mathbf{i}, \mathbf{k} \in \mathbb{N}_0^D$ *such that* $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = \Psi_{\mathbf{i}',\mathbf{k}'}^{D-s,\mathbf{j}'} \otimes \Psi_{0,0}^{s,0}$ *for some* $\mathbf{j}', \mathbf{i}', \mathbf{k}' \in \mathbb{N}_0^{D-s}$*. Then*

$$A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = A(L-1,d-1)\Psi_{\mathbf{i}',\mathbf{k}'}^{(d-1)s,\mathbf{j}'}.$$

*Proof.* Straightforward calculations yield

$$\begin{aligned}
A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} &= \sum_{\mathbf{l}\in Q(L,d)} \bigotimes_{n=1}^{d-1} \Delta_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n} \otimes \Delta_{l_d}^{(d)}\, \mathbf{1}_{[0,1)^s} \\
&= \sum_{\mathbf{l}\in Q(L-1,d-1)} \bigotimes_{n=1}^{d-1} \Delta_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n} \otimes \Delta_{1}^{(d)}\, \mathbf{1}_{[0,1)^s} \\
&= \sum_{\mathbf{l}\in Q(L-1,d-1)} \bigotimes_{n=1}^{d-1} \Delta_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n} \\
&= A(L-1,d-1)\Psi_{\mathbf{i}',\mathbf{k}'}^{(d-1)s,\mathbf{j}'}.
\end{aligned}$$

□

By simple induction we get the following corollary.

**Corollary 4.2.6.** *Consider* $\mathbf{j}, \mathbf{i}, \mathbf{k} \in \mathbb{N}_0^D$ *such that the function* $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$ *has* $d - t > 0$ *active blocks. Let* $\mathbf{j}', \mathbf{i}', \mathbf{k}' \in \mathbb{N}^{(d-t)s}$ *be the vectors* $\mathbf{j}, \mathbf{i}, \mathbf{k}$ *where the coordinates from the inactive* $t$ *blocks are removed. Then*

$$A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = A(L-t,d-t)\Psi_{\mathbf{i}',\mathbf{k}'}^{(d-t)s,\mathbf{j}'}$$

**Lemma 4.2.7.** *Let* $L \geq d$*. The algorithm* $A(L,d)$ *is exact on* $V^{D,L-d}$*.*

*Proof.* Due to ($\omega$-wise) linearity of the algorithm it suffices to prove the exactness of $A(L,d)$ on all the wavelets $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}, |\,\mathbf{j}\,| \leq L-d$. Fix one such function. The case $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} \equiv 1$ follows by the fact that all the weights used by $A(L,d)$ add up to 1, see Remark 4.2.1. Suppose now that all the blocks of $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$ are active. We are using the representation (3.4)

$$A(L,d) = \sum_{L-d+1 \leq |\,\mathbf{l}\,| \leq L} (-1)^{L-|\,\mathbf{l}\,|} \binom{d-1}{L-|\,\mathbf{l}\,|} \bigotimes_{n=1}^{d} U_{l_n}^{(n)}. \tag{4.3}$$

Recall the definitions of a $(0,m,s)$-net and of the QMC quadratures $U_l^{(n)}$ from Section 4.2.1. It is a simple observation that for $l' > l$ the algorithm $U_{l'}^{(k)}$ is exact on $V^{s,l}$. Take any $\mathbf{l}$ over which we are summing up in the above formula. Since $\sum_{n=1}^d l_n \geq L-d+1$ and $\sum_{n=1}^d |\,\mathbf{j}_n\,| \leq L-d$ there exists at least one index $\mu$ for which $l_\mu > |\,\mathbf{j}_\mu\,|$ and so $U_{l_\mu}^{(\mu)}\Psi_{\mathbf{i}_\mu,\mathbf{k}_\mu}^{s,\mathbf{j}_\mu} = 0$. Hence $A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = 0$, which is the exact value of the integral of $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$.

If $\mathbf{j}$ admits $t < d$ inactive blocks we may use Corollary 4.2.6 and the above argument applied to $A(L-t,d-t)$. □

**Lemma 4.2.8.** *Let* $(U_l^{(n)})_{l\in\mathbb{N}}$ *for every* $n = 1,\ldots,d$*, be a sequence of independent quadratures based on scrambled nets in base* $b$*. If* $\mathbf{j} \neq \mathbf{j}'$ *or if* $\mathbf{k} \neq \mathbf{k}'$*, then for every* $l, l' \in \mathbb{N}$

$$\mathbf{E}\left[U_l^{(n)}\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}}U_{l'}^{(n)}\Psi_{\mathbf{i}',\mathbf{k}'}^{s,\mathbf{j}'}\right] = 0. \tag{4.4}$$

*As a result, if either* $\mathbf{j} \neq \mathbf{j}'$ *or* $\mathbf{k} \neq \mathbf{k}'$*, for any* $L \geq d$ *the Smolyak method* $A(L,d)$ *basing on building blocks* $(U_l^{(n)})_{l\in\mathbb{N},n\in[d]}$ *satisfies*

$$\mathbf{E}\left[A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}A(L,d)\Psi_{\mathbf{i}',\mathbf{k}'}^{D,\mathbf{j}'}\right] = 0. \tag{4.5}$$

*Proof.* If $l \neq l'$, identity (4.4) follows by the independence of $U_l^{(n)}$ and $U_{l'}^{(n)}$. If $l = l'$ then (4.4) follows from [91, Lemma 4]. Now (4.5) may be easily deduced using representation (3.4).

□

**Lemma 4.2.9.** *Let* $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$, $\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}}$ *be two (not necessarily different) wavelets and for* $L \geq d$ *let* $A(L,d)$ *be the Smolyak method as in Definition 3.3.1, where for every* $n = 1,\ldots,d, l \in \mathbb{N}$*, the building block* $U_l^{(n)}$ *is an RQMC quadrature based on a scrambled* $(0,l-1,s)$*-net and*

*all the building blocks are randomized independently. Then there exists a constant $C$ which does not depend on $L$, such that*

$$\mathbf{E}\left(\left[(I_D - A(L,d))\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}\right]\left[(I_D - A(L,d))\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}}\right]\right) \leq C|\,\mathbf{j}\,|^{d-1}b^{-L}.$$

*Proof.* The case $u(\mathbf{j}) = \emptyset$ is trivial so without loss of generality we may assume $u(\mathbf{j}) \neq \emptyset$. Since $u(\mathbf{j}) \neq \emptyset$ we have $I_D\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = 0$ and so

$$\mathbf{E}\left(\left[(I_D - A(L,d))\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}\right]\left[(I_D - A(L,d))\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}}\right]\right) = \mathbf{E}\left[A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}A(L,d)\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}}\right].$$

By Cauchy-Schwarz inequality

$$\mathbf{E}\left[A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}A(L,d)\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}}\right] \leq \mathbf{E}\left[(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right]^{\frac{1}{2}}\mathbf{E}\left[(A(L,d)\Psi_{\mathbf{i}',\mathbf{k}}^{D,\mathbf{j}})^2\right]^{\frac{1}{2}},$$

so it suffices to show $\mathbf{E}\left[(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right] \leq C|\mathbf{j}|^{d-1}b^{-L}$.

We shall now proceed by induction on $(L,d)$ starting with $(L,1)$ for some $L \in \mathbb{N}$, and then moving from $(L-1,d-1)$ to $(L,d)$. For induction start, in the case $L = 1$ we have

$$\mathbf{E}\left[(A(1,1)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right] = \|\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}\|_{L^2} = 1.$$

Let $L > 1$. $A(L,1)$ is just a scrambled $(0, L-1, D)-$net quadrature, so it is exact on $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}$ for $|\,\mathbf{j}\,| \leq L-1$ . Let now $|\,\mathbf{j}\,| > L-1$. By Lemma 3 from [55]

$$\mathbf{E}\left[(A(L,1)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right] = N(L,1)^{-1}\Gamma_{\mathbf{j}} \leq b^{1-L},$$

where $N(L,1) = b^{L-1}$ is the number of evaluation points used and $\Gamma_{\mathbf{j}}$ is an appropriate gain coefficient which by Lemma 6 from [55] is bounded from above by 1. This proves the claim for $d = 1$.

Let us note that in the induction step we may confine ourselves to wavelets with all the blocks active. Indeed, let $\mathbf{j}$ be such that it admits $d - t > 0$ active blocks. Corollary 4.2.6 and our induction hypothesis yield

$$\mathbf{E}\left[(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right] = \mathbf{E}\left[(A(L-t,d-t)\Psi_{\mathbf{i}',\mathbf{k}'}^{(d-t)s,\mathbf{j}'})^2\right] \leq$$
$$C_1|\,\mathbf{j}'\,|^{d-t-1}b^{-L+t} \leq C|\,\mathbf{j}'\,|^{d-1}b^{-L},$$

($\mathbf{j}', \mathbf{i}', \mathbf{k}'$ have the same meaning as in Corollary 4.2.6). Now we may go over to the proof of the induction step assuming that we always deal only with functions with all the blocks active.

Note that for many $\mathbf{l} \in \mathbb{N}_0^d$ it holds a.s. that $\left(\bigotimes_{n=1}^d U_{l_n}^{(n)}\right) \Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}} = 0$ and all the vectors $\mathbf{l}$ for which this is not the case are contained in the set $S_{\mathbf{j}} = \bigcup_{\mu \geq d} S_{\mathbf{j},\mu}$, where $S_{\mathbf{j},\mu}$ is defined as

$$S_{\mathbf{j},\mu} := \{\mathbf{l} \in \mathbb{N}^d \,|\, |\mathbf{l}| = \mu, \forall_{n=1,\ldots,d}\, l_n \leq |\,\mathbf{j}_n\,|\}.$$

A justification of the inclusion is the following: suppose that for some $t$ we have $l_t > |\,\mathbf{j}_t\,|$. Integrating every (active) block yields 0. Exactness of $U_{l_t}^{(t)}$ on $\Psi_{\mathbf{i}_t,\mathbf{k}_t}^{s,\mathbf{j}_t}$ gives $U_{l_t}^{(t)} \Psi_{\mathbf{i}_t,\mathbf{k}_t}^{s,\mathbf{j}_t} = 0$.

We have

$$|S_{\mathbf{j},\mu}| \leq \binom{|\mathbf{j}| - \mu + d - 1}{d-1}.$$

That is because basically one asks, in how many ways one can distribute the 'overshoot' of $|\mathbf{j}| - \mu$ elements between $d$ coordinates.

By [55, Theorem 4, Lemma 6] we have for a constant $C_{s,d,b}$ not depending on $l$

$$\mathbf{E}[(U_l^{(n)} \Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})^2] \leq C_{s,d,b} b^{-l}.$$

Calling upon the representation (3.4) and using Lemma 4.2.8 we finally obtain with a generic constant $C$:

$$\begin{aligned}
\mathbf{E}\left[(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}})^2\right] &= \mathbf{E}\left[\left(\sum_{L-d+1 \leq |\mathbf{l}| \leq L} (-1)^{L-|\mathbf{l}|} \binom{d-1}{L-|\mathbf{l}|} \bigotimes_{n=1}^d U_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right)^2\right] \\
&\leq \max_{\mathbf{l}} \binom{d-1}{L-|\mathbf{l}|}^2 \mathbf{E}\left[\sum_{L-d+1 \leq |\mathbf{l}| \leq L} \left(\bigotimes_{n=1}^d U_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right)^2\right] \\
&\leq C\, \mathbf{E}\left[\sum_{L-d+1 \leq |\mathbf{l}| \leq L} \left(\bigotimes_{n=1}^d U_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right)^2\right] \\
&\leq C \sum_{\mu=L-d+1}^{L} \sum_{\mathbf{l} \in S_{\mathbf{j},\mu}} \prod_{n=1}^d \mathbf{E}\left[U_{l_n}^{(n)} \Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right]^2 \\
&\leq C \sum_{\mathbf{l} \in S_{\mathbf{j},L-d+1}} b^{-L} \\
&\leq C \binom{|\,\mathbf{j}\,| + 2d - 2 - L}{d-1} b^{-L} \leq C |\,\mathbf{j}\,|^{d-1} b^{-L}
\end{aligned}$$

□

Recall the definition of vector $\Psi^\alpha$ from Section 4.2.2. For a randomized operator $A : \Omega \to L(\mathcal{H}_\alpha^D, \mathbb{R})$, see Definition 3.2.1, we put

$$\Lambda_A := \mathbf{E}\left[((I_D - A)\Psi^\alpha)((I_D - A)\Psi^\alpha)^T\right], \tag{4.6}$$

where the operator $(I_D - A)$ is applied to the vector $\Psi^\alpha$ componentwise. It has been shown in [55, Theorem 1] that if $A$ is a randomized quadrature applied to integrands from $\mathcal{H}^D_\alpha$, it holds

$$e^{\mathrm{r}}(I_D, A) = \sqrt{\rho(\Lambda_A)},$$

where $\rho(\Lambda_A)$ denotes the spectral radius of $\Lambda_A$, i.e. the largest absolute value of eigenvalues of $\Lambda_A$. Put

$$\Lambda := \Lambda_{A(L,d)}. \tag{4.7}$$

**Remark 4.2.10.** By Lemma 4.2.8 $\Lambda$ is a block diagonal matrix consisting of $b^{|u(\mathbf{j})|} \times b^{|u(\mathbf{j})|}$ blocks $\Lambda(\mathbf{j}, \mathbf{k})$ given by

$$\Lambda(\mathbf{j}, \mathbf{k}) = \mathbf{E}[((I_D - A(L,d))\Psi^{D,\mathbf{j},\alpha}_{\mathbf{i},\mathbf{k}})_{\mathbf{i}\in\theta_\mathbf{j}}((I_D - A(L,d))\Psi^{D,\mathbf{j},\alpha}_{\mathbf{i},\mathbf{k}})^T_{\mathbf{i}\in\theta_\mathbf{j}}].$$

For $u(\mathbf{j}) = \emptyset$ we have $\Lambda(\mathbf{j}, \mathbf{k}) = 0 \in \mathbb{R}^{1\times 1}$. For $u(\mathbf{j}) \neq \emptyset$ it holds $I_D\Psi^{D,\mathbf{j},\alpha}_{\mathbf{i},\mathbf{k}} = 0$ and consequently

$$\Lambda(\mathbf{j}, \mathbf{k}) = \mathbf{E}[(A(L,d)\Psi^{D,\mathbf{j},\alpha}_{\mathbf{i},\mathbf{k}})_{\mathbf{i}\in\theta_\mathbf{j}}(A(L,d)\Psi^{D,\mathbf{j},\alpha}_{\mathbf{i},\mathbf{k}})^T_{\mathbf{i}\in\theta_\mathbf{j}}].$$

Due to the block diagonal structure the eigenvalues of $\Lambda$ are exactly the eigenvalues of all the blocks, i.e.

$$e^{\mathrm{r}}(I_D, A(L,d))^2 = \sup_{\mathbf{j},\mathbf{k}} \rho(\Lambda(\mathbf{j}, \mathbf{k}))$$

**Theorem 4.2.11.** *Let $\alpha > \frac{1}{2}, s, d \in \mathbb{N}, D = sd$. For $n = 1, \ldots, d$, and $l \in \mathbb{N}$ let $U^{(n)}_l$ be randomized QMC quadratures based on scrambled $(0, l-1, s)$-nets in base $b$. Let $A(L,d)$ denote the corresponding Smolyak method approximating the integral $I_D$, where the building blocks $(U^{(n)}_l)_{l,n}$ are all randomized independently, and denote by $N$ the number of function evaluations performed by $A(L,d)$. Then there exists a constant $C$ not depending on $N$ such that the randomized error satisfies*

$$e^{\mathrm{r}}(I_D, A(L,d)) \leq C\frac{\log(N)^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}.$$

**Remark 4.2.12.** Note that using the bounds for errors of quadratures based on scrambled $(0, m, s)$-nets from [55] and then applying the general Theorem 3.5.4 yields a weaker asymptotic bound with exponent $(d-1)(\frac{3}{2} + \alpha)$ in the logarithmic term.

**Remark 4.2.13.** In Example 3.5.6 we have argued that the cardinality of information used by the Smolyak method $\widetilde{A}(L,d)$ based on $\widetilde{U}^{(n)}_l, n = 1, \ldots, d, l \in \mathbb{N}$, where $\widetilde{U}^{(n)}_l$ is a quadrature based on a $(0, l, s)$-net is of the order $\Theta(b^L L^{d-1})$. Obviously this estimate carries over to the situation described in this chapter, changing the level of the nets used by 1 ($U^{(n)}_l$ is based on $(0, l-1, s)$-net instead of $(0, l, s)$-net) changes only the implicit constant.

*Proof of Theorem 4.2.11.* By Lemma 4.2.9 the entries of $\Lambda(\mathbf{j},\mathbf{k})$ are of the order $b^{-2\alpha|\,\mathbf{j}\,|}|\,\mathbf{j}\,|^{d-1}b^{-L}$. Due to the exactness result from Lemma 4.2.7 we only have to consider blocks for which $|\,\mathbf{j}\,| > L-d \approx L$, since for other $\mathbf{j}$ the blocks $\Lambda(\mathbf{j},\mathbf{k})$ consist just of zeros. For any square matrix $D=(d_{i,j})_{i,j=1}^n$ all the eigenvalues lie inside $\bigcup_{i=1}^n K_i$, where

$$K_i = \{z\in\mathbb{C}\,|\,|z-d_{i,i}|\le\sum_{j\neq i}|d_{i,j}|\}$$

are Gershgorin circles. Taking into account Remark 4.2.10 we have with a generic constant $C$:

$$\begin{aligned} e^{\mathrm{r}}(I_D,A(L,d))^2 &= \sup_{\mathbf{j},\mathbf{k}}\rho(\Lambda(\mathbf{j},\mathbf{k})) \\ &\le \sup_{|\,\mathbf{j}\,|>L-d} Cb^{|u(\mathbf{j})|}b^{-2\alpha|\,\mathbf{j}\,|}|\,\mathbf{j}\,|^{d-1}b^{-L} \\ &\le \sup_{|\,\mathbf{j}\,|>L-d} Cb^{D}b^{-2\alpha|\,\mathbf{j}\,|}|\,\mathbf{j}\,|^{d-1}b^{-L} \\ &\le Cb^{-L(1+2\alpha)}L^{d-1} \end{aligned}$$

To justify the last inequality it is enough to show that for some $\tilde{C}$ not depending on $L$ we have

$$\sup_{\mathbf{j}:|\,\mathbf{j}\,|>L-d} b^{2\alpha(L-|\,\mathbf{j}\,|)}\left(\tfrac{|\,\mathbf{j}\,|}{L}\right)^{d-1}\le\tilde{C}. \tag{4.8}$$

To this end consider $f:\mathbb{R}_{>0}\to\mathbb{R}, x\mapsto b^{2\alpha(L-x)}\left(\frac{x}{L}\right)^{d-1}$. It holds

$$f'(x) = b^{2\alpha(L-x)}\left(\tfrac{x}{L}\right)^{d-2}\left[-2\alpha\tfrac{x}{L}\log(b)+\tfrac{d-1}{L}\right],$$

and so $f$ attains its (sole) local maximum at $x_0=\frac{d-1}{2\alpha\log(b)}$. Therefore

$$\begin{aligned} &\sup_{\mathbf{j}:|\,\mathbf{j}\,|>L-d} b^{2\alpha(L-|\,\mathbf{j}\,|)}\left(\tfrac{|\,\mathbf{j}\,|}{L}\right)^{d-1}\le b^{2\alpha d}\left(\tfrac{d-1}{2\alpha\log(b)L}\right)^{d-1} \\ &\le b^{2\alpha d}\left(\tfrac{1}{2\alpha\log(b)}\right)^{d-1}\le(2b)^{2\alpha d}, \end{aligned}$$

which proves the desired inequality.

By Remark 4.2.13

$$N=\mathcal{O}(b^L L^{d-1}).$$

It follows

$$b^{-L(1+2\alpha)}L^{d-1}=\frac{L^{(d-1)(2+2\alpha)}}{b^{L(1+2\alpha)}L^{(d-1)(1+2\alpha)}}=\mathcal{O}\left(\left(\frac{(\log(N))^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}\right)^2\right).$$

Hence we have

$$e^{\mathrm{r}}(I_D,A(L,d))\le C\frac{(\log(N))^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}.$$

□

### 4.2.4 Lower Bounds on the Integration Error

**Lemma 4.2.14.** *There exists a constant $c_{b,s}$ independent of $l \in \mathbb{N}$ such that for every $\mathbf{j} \in \mathbb{N}^s$ with $|\,\mathbf{j}\,| \geq l + s - 1$ and every admissible $\mathbf{i}, \mathbf{k}$ it holds*

$$\mathbf{E}\left[(U_l \Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})^2\right] = c_{b,s} b^{-l},$$

*where $U_l$ denotes an arbitrary QMC quadrature based on a scrambled $(0, l-1, s)$-net in base $b$.*

*Proof.* For $l, \Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}}$, as above and $x \in \operatorname{supp}(\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})$ we have

$$\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}}(x) = \prod_{t=1}^{s} b^{\frac{j_t - 2}{2}} \gamma_t(x),$$

where $\gamma_t(x) \in \{b-1, -1, b\}$. It follows that $|\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}}(x)| = \gamma(x) b^{\frac{|\mathbf{j}|}{2} - s}$, with $\gamma(x) = \prod_{t=1}^{s} |\gamma_t(x)|$. Put $\overline{\gamma} = |\operatorname{supp}(\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})|^{-1} \int_{\operatorname{supp}(\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})} \gamma(x)^2 \, dx$. Now, since $|\,\mathbf{j}\,| \geq l + s - 1$, at most one point of the net used by $U_l$ falls into $\operatorname{supp}(\Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})$ and this happens with probability $b^{l-|\mathbf{j}|}\rho(\mathbf{j})$, where $1 \leq \rho(\mathbf{j}) \leq b^{s-1}$. Denoting by $(p_t)_{t=1}^{b^{l-1}}$ the scrambled net used by $U_l$ we get

$$\begin{aligned}
\mathbf{E}\left[(U_l \Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}})^2\right] &= b^{-2l+2}\, \mathbf{E}\left[\left(\sum_{t=1}^{b^{l-1}} \Psi_{\mathbf{i},\mathbf{k}}^{s,\mathbf{j}}(p_t)\right)^2\right] \\
&= b^{-2l+2} b^{l-|\mathbf{j}|} \rho(\mathbf{j}) b^{|\mathbf{j}|-2s} \overline{\gamma} = c_{b,s} b^{-l}.
\end{aligned}$$

□

**Lemma 4.2.15.** *Let $d, L \in \mathbb{N}, \mathbf{j} = \left(\lfloor \frac{2L}{d} \rfloor, \lfloor \frac{2L}{d} \rfloor, \ldots, \lfloor \frac{2L}{d} \rfloor, 2L - (d-1)\lfloor \frac{2L}{d} \rfloor\right) \in \mathbb{N}^d$ and*

$$S_{\mathbf{j},L} = \{\mathbf{l} \in \mathbb{N}^d \,|\, |\mathbf{l}| = L, \forall_{n=1,\ldots,d}\, l_n \leq |\,\mathbf{j}_n\,|\}.$$

*It holds*

$$|S_{\mathbf{j},L}| = \Omega(L^{d-1}),$$

*where the implicit constant may depend on $d$.*

*Proof.* For the ease of presentation we shall prove only the case when $d$ divides $2L$. After obvious changes the proof goes through in the general case. So let $\mathbf{j} = \left(\frac{2L}{d}, \ldots, \frac{2L}{d}\right)$. Moreover, since we are interested in asymptotic statement for $L$ we may without loss of generality assume that $L \geq \frac{d(d-1)}{2}$. One may describe the situation in the following way: we have $d$ bins numbered $1, 2, \ldots, d$, each of them with capacity $\frac{2L}{d}$. How many ways are there to arrange $L$ indistinguishable balls in those bins? Let us focus on the bins with numbers $1, \ldots, d-1$. Any of them may have any number of balls between $\frac{(d-2)L}{d(d-1)}$ and $\frac{dL}{d(d-1)} - 1$ independently of all the other bins with numbers $1, \ldots, d-1$. Indeed, if every

of those bins has $\frac{(d-2)L}{d(d-1)}$ balls then putting in the $d$-th bin $\frac{2L}{d}$ balls we end up with $L$ balls altogether. On the other hand, if every of the first $d-1$ bins has $\frac{dL}{d(d-1)}-1$ balls then putting $d-1$ balls in the $d$-th bin we also end up with $L$ balls altogether. That is,

$$|S_{\mathbf{j},L}| \geq \left(\frac{dL-(d-2)L}{d(d-1)}\right)^{d-1} = \left(\frac{2L}{d(d-1)}\right)^{d-1} = \Omega(L^{d-1}).$$

□

**Theorem 4.2.16.** *Let $\alpha > \frac{1}{2}, d, s \in \mathbb{N}, D = sd$. For $n = 1, \dots d$, and $l \in \mathbb{N}$, let $U_l^{(n)}$ be independently randomized QMC quadratures based on scrambled $(0, l-1, s)$-nets. Let $A(L,d)$ denote the corresponding Smolyak method approximating the integral $I_D$. Then there exists a constant $c_{s,b}$ depending on $s$ and $b$ such that the randomized error expressed in terms of the cardinality of function evaluations $N$ satisfies*

$$e^{\mathrm{r}}(I_D, A(L,d)) \geq c_{s,b}\frac{(\log(N))^{(d-1)(1+\alpha)}}{N^{\alpha+\frac{1}{2}}}.$$

*Proof.* Recall the definition of $\Lambda$ from (4.7). Remark 4.2.13 gives $N = \Omega(b^L L^{d-1})$. Due to Remark 4.2.10 it suffices to show that

$$\sup_{\mathbf{j},\mathbf{k}} \rho(\Lambda(\mathbf{j},\mathbf{k})) \geq c b^{-L(1+2\alpha)} L^{d-1}, \tag{4.9}$$

with a constant $c > 0$ not depending on $L$, where $\Lambda(\mathbf{j},\mathbf{k})$ is the block of $\Lambda$ corresponding to $\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}, \mathbf{i} \in \theta_{\mathbf{j}}$.

To ascertain that $\sup_{\mathbf{j},\mathbf{k}} \rho(\Lambda(\mathbf{j},\mathbf{k})) \geq c b^{-L(1+2\alpha)} L^{d-1}$ it is enough to show that for some $\tilde{c} > 0$ independent of $L$ and some $\mathbf{j},\mathbf{k}$, every diagonal entry of $\Lambda(\mathbf{j},\mathbf{k})$ is bounded from below by $\tilde{c} b^{-L(1+2\alpha)} L^{d-1}$. Indeed, if this holds then the same bound holds also for the trace of $\Lambda(\mathbf{j},\mathbf{k})$, and so for $\rho(\Lambda(\mathbf{j},\mathbf{k}))$. That is, we need to show that for appropriate $\mathbf{j}$ with $|\,\mathbf{j}\,|$ proportional to $L$ we have

$$\mathbf{E}\left[\left(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}\right)^2\right] \geq \tilde{c} b^{-L} L^{d-1}.$$

We take $\mathbf{j} = \left(\lfloor\frac{2L}{d}\rfloor, \lfloor\frac{2L}{d}\rfloor, \dots, \lfloor\frac{2L}{d}\rfloor, 2L-(d-1)\lfloor\frac{2L}{d}\rfloor\right)$. Putting

$$S_{\mathbf{j},L} := \{\mathbf{l} \in \mathbb{N}^d \,|\, |\mathbf{l}| = L, \forall_{n=1,\dots,d}\, l_n \leq |\,\mathbf{j}_n\,|\}$$

and recalling from Lemma 4.2.15 that $|S_{\mathbf{j},L}| = \Omega(L^{d-1})$ we obtain for $L$ large enough

$$\begin{aligned}
&\mathbf{E}\left[\left(A(L,d)\Psi_{\mathbf{i},\mathbf{k}}^{D,\mathbf{j}}\right)^2\right] = \mathbf{E}\left[\left(\sum_{\max\{d,L-d+1\}\leq|\mathbf{l}|\leq L}(-1)^{L-|\mathbf{l}|}\binom{d-1}{L-|\mathbf{l}|}\bigotimes_{n=1}^{d} U_{l_n}^{(n)}\Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right)^2\right] \\
&= \mathbf{E}\left[\sum_{\mu=L-d+1}^{L}\sum_{\mathbf{l}\in S_{\mathbf{j},\mu}}\binom{d-1}{L-\mu}^2\left(\bigotimes_{n=1}^{d} U_{l_n}^{(n)}\Psi_{\mathbf{i}_n,\mathbf{k}_n}^{s,\mathbf{j}_n}\right)^2\right] \\
&\geq C\sum_{\mu=L-d+1}^{L}|S_{\mathbf{j},\mu}|b^{-\mu} \geq C|S_{\mathbf{j},L}|b^{-L} \geq CL^{d-1}b^{-L},
\end{aligned}$$

where the first inequality follows by Lemma 4.2.14 and the second inequality by Lemma 4.2.15. □

# Chapter 5

# On Negatively Dependent Sampling Schemes, Variance Reduction, and Probabilistic Upper Discrepancy Bounds

## 5.1 Introduction

Plain Monte Carlo (MC) sampling is a method frequently used in stochastic simulation and multivariate numerical integration. Let $p_1, \ldots, p_N$, be independent random points, each uniformly distributed in the $d$-dimensional unit cube $[0,1)^d$. For an arbitrary integrable random variable (or function) $f : [0,1)^d \to \mathbb{R}$ we consider the MC estimator (or quadrature)

$$\mu^{\mathrm{MC}} f = \frac{1}{N} \sum_{i=1}^{N} f(p_i) \tag{5.1}$$

for the expected value (or integral)

$$If = \int_{[0,1)^d} f(x)\, dx.$$

An advantage of the MC estimator is that already under the very mild assumption on $f$ to be square integrable, it converges to $If$ for $N \to \infty$ with convergence rate $1/2$. Even though the convergence rate is not very impressive, it has the invaluable advantage that it does not depend on the number of variables $d$.

However, there are many dependent sampling schemes (i.e., random sample points $p_i$, $i = 1, \ldots, N$, that are still uniformly distributed in $[0,1)^d$, but not necessarily independent any more) known that are superior to plain MC sampling with respect to certain objectives. An example are suitably randomized quasi-Monte Carlo (RQMC) point sets. They ensure, for instance, higher convergence rates for numerical integration of sufficiently smooth functions, they lead to much smaller asymptotic discrepancy

measures, their sample points do not tend to cluster and have more evenly distributed lower-dimensional projections (see, e.g., [18, 20, 71, 75]). It would be desirable to be able to construct dependent sampling schemes that have some of these or other favorable properties, and that are, with respect to other objectives, at least as good as MC sampling schemes.

Recently, in this direction some research had been done. In [72] Christiane Lemieux showed that a negative dependence property of RQMC points ensures that the variance of the corresponding RQMC estimator for functions $f$ that are monotone with respect to each variable is never larger than the variance of the corresponding MC estimator $\mu^{\mathrm{MC}} f$. She also proved that a different negative dependence property yields that the variance of the RQMC estimator for an arbitrary bounded quasimonotone $f$ is never larger than the variance of $\mu^{\mathrm{MC}} f$. Those negative dependence properties rely solely on the marginals and the bivariate copulas of the RQMC points (i.e., on the distribution of single points and on the common distribution of pairs of points).

In a different line of research it has been shown in [41, 53] that a specific negative dependence property of RQMC points guarantees that they satisfy the same pre-asymptotic probabilistic discrepancy bounds (with explicitly revealed dependence on the number of points $N$ as well as on the dimension $d$) as MC points. Here the negative dependence property relies on the common distribution of all sample points. Related results can be found in [21].

For more extensive motivations of both lines of research we refer to the elaborate introductions of [72] and [21, 41], respectively. The aim of this chapter is to survey and compare the approaches mentioned above and to provide several new results.

This chapter is organized as follows: In Section 5.2 we introduce some notions of negatively dependent sampling schemes and discuss how one can benefit from them. In Section 5.3 we provide new probabilistic upper discrepancy bounds for sampling schemes. The discrepancy measures we consider are the star discrepancy and the weighted star discrepancy. These bounds are "plug-in results" in the following sense: One just has to check whether a sampling scheme satisfies the sufficient negative dependence condition and – if this is the case – one obtains immediately a probabilistic discrepancy bound with explicitly given constants. In Section 5.4, we give several examples of sampling schemes that satisfy the one or the other notion of negative dependence, including a generalized notion of stratified sampling schemes, mixed randomized sequences and randomly shifted and jittered rank-1 lattices. Finally, in Section 5.5 we elaborate on relations between different notions of negative dependence.

We finish the introduction by stating some notation. Let $d, N \in \mathbb{N}$. If not stated otherwise we are always considering a randomized point set $(p_j)_{j=1}^N := \mathcal{P} \subset [0,1)^d$ consisting of $N$ points. For $a, b \in \mathbb{R}^d, a = (a_1, \ldots, a_d), b = (b_1, \ldots, b_d)$, we write $a \leq b$ if $a_i \leq b_i, i = 1, \ldots, d$. All other inequalities are also to be understood componentwise. Moreover, $[a, b) := [a_1, b_1) \times \ldots \times [a_d, b_d)$. Via $\mathcal{C}_0^d$ we denote the set of boxes ("corners") anchored at 0

$$\mathcal{C}_0^d := \{[0, a) \,|\, a \in [0,1)^d\},$$

and by $\mathcal{C}_1^d$ the set of boxes anchored at 1,

$$\mathcal{C}_1^d := \{[a,1) \,|\, a \in [0,1)^d\}.$$

We write $\mathcal{D}_0^d$ for the set of differences of boxes anchored at 0,

$$\mathcal{D}_0^d := \{Q \setminus R \,|\, Q, R \in \mathcal{C}_0^d\}.$$

For $m \in \mathbb{N}$ we denote the set $\{1, 2, \ldots, m\}$ by $[m]$, $\lambda^d$ stands for the d-dimensional Lebesgue measure on $\mathbb{R}^d$, in case $d = 1$ we just write $\lambda$. If not specified, all random variables are defined on a probability space $(\Omega, \Sigma, \mathbf{P})$.

## 5.2 Review of Notions of Negative Dependance of Sampling Schemes

### 5.2.1 $\gamma$-Negative Dependence of Binary Random Variables and Sampling Schemes

The concept of negative dependence was introduced by Lehmann [70] for pairs of random variables. In the literature one finds several contributions on rather demanding notions of negative dependence, such as, e.g., negative association introduced in [64]; a survey can be found in [94]. Sufficient for our purpose is the following notion for *Bernoulli* or *binary random variables*, i.e., random variables that only take values in $\{0, 1\}$.

**Definition 5.2.1.** Let $\gamma \geq 1$. We call binary random variables $T_1, T_2, \ldots, T_N$ *upper $\gamma$-negatively dependent* if

$$\mathbf{P}\left(\bigcap_{j \in u} \{T_j = 1\}\right) \leq \gamma \prod_{j \in u} \mathbf{P}(T_j = 1) \quad \text{for all } u \subseteq [N], \tag{5.2}$$

and *lower $\gamma$-negatively dependent* if

$$\mathbf{P}\left(\bigcap_{j \in u} \{T_j = 0\}\right) \leq \gamma \prod_{j \in u} \mathbf{P}(T_j = 0) \quad \text{for all } u \subseteq [N]. \tag{5.3}$$

We call $T_1, T_2, \ldots, T_N$ *$\gamma$-negatively dependent* if both conditions (5.2) and (5.3) are satisfied. If $\gamma = 1$, we usually suppress the explicit reference to $\gamma$.

1-negative dependence is usually called negative orthant dependence, cf. [10].

Notice that, in particular, independent binary random variables are negatively dependent. Furthermore, it is easily seen that for $N = 2$ and $\gamma = 1$ the notions of upper and lower $\gamma$-negative dependence are equivalent, cf. [70].

We are interested in binary random variables $T_i$, $i = 1, \ldots, N$, of the form $T_i = \mathbf{1}_A(p_i)$, where $A$ is a Lebesgue-measurable subset of $[0,1)^d$ (whose characteristic function is denoted by $\mathbf{1}_A$), and $p_1, \ldots, p_N$ are randomly chosen points in $[0,1)^d$.

We will use the following bound of Hoeffding-type; for a proof see, e.g., [53].

**Theorem 5.2.2.** *Let $\gamma \geq 1$, and let $T_1, \ldots, T_N$ be $\gamma$-negatively dependent binary random variables. Put $S := \sum_{i=1}^{N}(T_i - \mathbb{E}[T_i])$. We have*

$$\mathbf{P}\left(|S| \geq t\right) \leq 2\gamma \exp\left(-\frac{2t^2}{N}\right) \quad \textit{for all } t > 0. \tag{5.4}$$

**Definition 5.2.3.** A randomized point set $\mathcal{P} = (p_j)_{j=1}^{N}$ is called a *sampling scheme* if every single $p \in \mathcal{P}$ is distributed uniformly in $[0,1)^d$ and the vector $(p_1, \ldots, p_N)$ is exchangeable, meaning that for any permutation $\pi$ of $[N]$ it holds that the law of $(p_1, \ldots, p_N)$ is the same as the law of $(p_{\pi(1)}, \ldots, p_{\pi(N)})$.

The assumption of exchangeability is only of technical nature and, if we consider $\mathcal{P}$ as a randomized point set, may be always obtained in the process of symmetrization. Indeed, let $\tilde{\mathcal{P}}$ be a randomized point set such that every $\tilde{p} \in \tilde{\mathcal{P}}$ is uniformly distributed in $[0,1)^d$ and let $\pi$ be a random uniformly chosen permutation of $[N]$. Then $(\tilde{p}_{\pi(1)}, \ldots, \tilde{p}_{\pi(N)})$ is already a sampling scheme.

### 5.2.2 Pairwise Negative Dependence and Variance Reduction

**Definition 5.2.4.** We say that a sampling scheme $\mathcal{P}$ is *pairwise negatively dependent* if for every $Q, R \in \mathcal{C}_1^d$ it holds that the random variables

$$\mathbf{1}_Q(p_1), \mathbf{1}_R(p_2)$$

are negatively dependent.

In other words, a sampling scheme $\mathcal{P}$ is pairwise negatively dependent if for every $Q, R \in \mathcal{C}_1^d$ we have

$$\mathbf{P}(p_1 \in Q, p_2 \in R) \leq \mathbf{P}(p_1 \in Q)\,\mathbf{P}(p_2 \in R), \tag{5.5}$$

$$\mathbf{P}(p_1 \notin Q, p_2 \notin R) \leq \mathbf{P}(p_1 \notin Q)\,\mathbf{P}(p_2 \notin R). \tag{5.6}$$

Note that (5.5) implies (5.6) and vice versa, therefore one of the conditions is in fact redundant. In [72] this is known as negatively upper orthant dependent - or NUOD - sampling schemes.

Our interest lies in numerical integration of functions from some class $\mathcal{F} \subset L^2([0,1)^d)$ using RQMC. A QMC quadrature is just a quadrature consisting of $N$ nodes, such that the evaluation in every node is given the same weight $\frac{1}{N}$. By randomizing the set of nodes we obtain an RQMC quadrature. Let $\mu_{\mathcal{P}} f$ be an RQMC estimator of $If := \int_{[0,1)^d} f(x)\,dx$ based on the sampling scheme $\mathcal{P} = (p_j)_{j=1}^{N}$, i.e.

$$\mu_{\mathcal{P}} f = \frac{1}{N}\sum_{j=1}^{N} f(p_j).$$

Moreover, let $\mu^{\mathrm{MC}} f$ be an estimator of $If$ based on a Monte Carlo sample consisting of $N$ points (i.e. the integration nodes are chosen independently and uniformly from $[0,1)^d$, see (5.1)).

It turns out that randomized QMC quadratures based on pairwise negatively dependent sampling schemes may lead to variance reduction in comparison to the simple MC quadratures. Here we describe shortly one of such cases, namely when integrands are bounded quasimonotone functions. The following exposition is based on [72].

To define what a quasimonotone function is we need first to introduce the notion of quasivolume. For $a, b \in [0,1)^d$, $J \subset [d]$ and a function $f : [0,1)^d \to \mathbb{R}$ we write $f(a_J, b_{-J})$ to represent the evaluation of $f$ at the point $(x_1, \ldots, x_d)$, where $x_j = a_j$ for $j \in J$ and $x_j = b_j$ otherwise. The quasivolume of $f$ over an interval $A = [a, b) \subset [0,1)^d$ is given by

$$\Delta^d(f, A) := \sum_{J \subset [d]} (-1)^{|J|} f(a_J, b_{-J}).$$

We say that the function $f$ is *quasimonotone* if

$$\Delta^d(f, A) \geq 0$$

for every interval $A$. Note that if we define a content $\nu_f([0, a)) := f(a), a \in [0,1)^d$, then quasimonotonicity of $f$ means exactly that for any axis-parallel rectangle $R \subset [0,1)^d$ it holds $\nu_f(R) \geq 0$.

Apart from pairwise negative dependence there are a few similar notions which are also of interest.

**Definition 5.2.5.** Let $\mathcal{P} = (p_j)_{j=1}^N$ be a sampling scheme in $[0,1)^d$. Put $p_j = (p_j^{(1)}, \ldots, p_j^{(d)})$, and for $i = 1, \ldots, d$, denote by $p^{(1:i-1)}$ the orthogonal projection of $p$ onto the first $i-1$ coordinates. If for every $i = 1, \ldots, d$, and every measurable $A, B \subset [0,1)^{i-1}, \alpha, \beta \in [0,1)$

$$\begin{aligned}&\mathbf{P}(p_1^{(i)} \geq \alpha, p_2^{(i)} \geq \beta | p_1^{(1:i-1)} \in A, p_2^{(1:i-1)} \in B) \\ &\leq \mathbf{P}(p_1^{(i)} \geq \alpha | p_1^{(1:i-1)} \in A, p_2^{(1:i-1)} \in B)\, \mathbf{P}(p_2^{(i)} \geq \beta | p_1^{(1:i-1)} \in A, p_2^{(1:i-1)} \in B),\end{aligned}$$

we say that $\mathcal{P}$ is *conditionally negatively quadrant dependent* (conditionally NQD).

Even stronger is the notion of coordinatewise independent NQD sampling scheme.

**Definition 5.2.6.** With the notation as in Definition 5.2.5, if $(p_1^{(i)}, p_2^{(i)})_{i=1}^d$ are independent for every $i = 1, \ldots, d$, and every $q, r \in [0,1)$ we have

$$\mathbf{P}(p_1^{(i)} \geq q, p_2^{(i)} \geq r) \leq \mathbf{P}(p_1^{(i)} \geq q)\, \mathbf{P}(p_2^{(i)} \geq r),$$

the sampling scheme $\mathcal{P}$ is called *coordinatewise independent NQD*.

Christiane Lemieux showed in [72, Corollary 2] that conditionally NQD sampling schemes provide RQMC estimators of integrals with variance no bigger then the variance of the MC estimator if the integrand is monotone in each coordinate.

The following is basically a combination of Proposition 3, Remark 8 and Corollary 2 from [72].

**Theorem 5.2.7.** *Let $f : [0,1)^d \to \mathbb{R}$ be square-integrable and $\mathcal{P}$ be a sampling scheme. Then if either*

1. *The function $f$ is bounded and $f$ or $-f$ is quasimonotone and $\mathcal{P}$ is pairwise negatively dependent,*
2. *The function $f$ is monotone in each coordinate and $\mathcal{P}$ is conditionally negatively quadrant dependent,*

*it holds*

$$\mathrm{Var}(\mu_{\mathcal{P}} f) \leq \mathrm{Var}(\mu^{\mathrm{MC}} f).$$

In Section 5.4 we present several sampling schemes exhibiting different notions of negative dependece. In Section 5.5 we discuss relations between the introduced notions of negative dependence.

Let us note that the aforementioned article provides actually more general results. Interested reader will find details in Sections 3 and 4 of [72].

### 5.2.3 Negatively Dependent Sampling Schemes and Discrepancy

**Definition 5.2.8.** Let $\mathcal{S}$ be a system of measurable subsets of $[0,1)^d$. We say that a sampling scheme $(p_j)_{j=1}^N = \mathcal{P}$ is $\mathcal{S} - \gamma-$*negatively dependent* if for every $Q \in \mathcal{S}$ the random variables

$$(\mathbf{1}_Q(p_j))_{j=1}^N$$

are $\gamma$-negatively dependent.

In other words for every $t \leq N$ we require

$$\mathbf{P}(\bigcap_{j=1}^{t} \{p_j \in Q\}) \leq \gamma \prod_{j=1}^{t} \mathbf{P}(p_j \in Q), \tag{5.7}$$

$$\mathbf{P}(\bigcap_{j=1}^{t} \{p_j \notin Q)\} \leq \gamma \prod_{j=1}^{t} \mathbf{P}(p_j \notin Q). \tag{5.8}$$

Note that differently from the case of pairwise negative dependence, for $N > 2$ one indeed needs to check both inequalities as they do not, in general, imply one another. If $\gamma = 1$ and $\mathcal{S} = \mathcal{C}_0^d$ we usually talk just of negatively dependent sampling schemes. Moreover, if (5.7) is satisfied we speak of upper $\gamma-$ negatively dependent sampling schemes and if (5.8) is satisfied we speak of lower $\gamma-$ negatively dependent sampling schemes.

Our interest in negative dependence comes from the fact that negatively dependent sampling schemes exhibit with high probability small discrepancy. For information on discrepancy ant its connection to numerical integration, see Section 2.3.

It has been shown in [41] that $\mathcal{D}_0^d$ - $\gamma$ - negatively dependent sampling schemes have with large probability star discrepancy of the order $\sqrt{\frac{d}{N}}$. More precisely the following theorem holds.

**Theorem 5.2.9.** *Let $d, N \in \mathbb{N}$ and $\rho \in [0, \infty)$. Let $\mathcal{P} = (p_j)_{j=1}^N$ be a negatively $\mathcal{D}_0^d$-$e^{\rho d}$-dependent sampling scheme.*
*Then for every $c > 0$*

$$D_N^*(\mathcal{P}) \leq c\sqrt{\frac{d}{N}} \tag{5.9}$$

*holds with probability at least $1 - e^{-(1.6741 \cdot c^2 - 10.7042 - \rho) \cdot d}$. Moreover, for every $\theta \in (0, 1)$*

$$\mathbf{P}\left( D_N^*(\mathcal{P}) \leq 0.7729\sqrt{10.7042 + \rho + \frac{\ln\left((1-\theta)^{-1}\right)}{d}}\sqrt{\frac{d}{N}} \right) \geq \theta. \tag{5.10}$$

Notice that these bounds depend only mildly on $\rho$ or $\gamma = e^{\rho d}$. Furthermore, $\mathcal{D}_0^d$-1-negatively dependent sampling schemes satisfy the same preasymptotic discrepancy bound as Monte Carlo point sets do. For more details see [41].

In Remark 5.4.21 we present a bound similar to (5.10) under a bit different assumptions that can be applied to so-called mixed randomized sequences.

## 5.3 New Probabilistic Discrepancy Bounds

### 5.3.1 Bound on the Star Discrepancy for Negatively Dependent Sampling Schemes

Proving that a given sampling scheme is $\mathcal{D}_0^d$-$\gamma$-negatively dependent may turn out to be a difficult task. One of the problems lies in the fact that elements of $\mathcal{D}_0^d$ may in general not be represented as Cartesian products of one-dimensional intervals, cf. also Remark 5.4.21. With this in mind we would like to weaken the assumptions on the sampling scheme $\mathcal{P}$. In the following result we show that by requiring the sampling scheme $\mathcal{P}$ only to be $\mathcal{C}_0^d$-$\gamma$-negatively dependent one already gets with high probability a discrepancy of the order $\sqrt{\frac{d}{N}\log(1 + \frac{N}{d})}$.

**Theorem 5.3.1.** *Let $d, N \in \mathbb{N}$ and $\rho \in [0, \infty)$. Let $\mathcal{P} = (p_j)_{j=1}^N$ be a $\mathcal{C}_0^d$-$e^{\rho d}$-negatively dependent sampling scheme in $[0, 1)^d$. Then for every $c > 0$*

$$D_N^*(\mathcal{P}) \leq c\sqrt{\frac{d}{N}\log\left(6e\left[1 + \frac{N}{d}\right]\right)} \tag{5.11}$$

*holds with probability at least $1 - 2e^{-(\frac{c^2}{2} - 1 - \rho)d}$. Moreover, for every $\theta \in (0, 1)$*

$$\mathbf{P}\left( D_N^*(\mathcal{P}) \leq \sqrt{\frac{2}{N}}\sqrt{d\log(\eta) + \rho d + \log\left(\frac{2}{1-\theta}\right)} \right) \geq \theta, \tag{5.12}$$

*where $\eta := \eta(N, d) = 6e\left(\max(1, \frac{N}{2d\log(6e)})\right)^{\frac{1}{2}}$.*

The proof of Theorem 5.3.1 requires some preparation. To "discretize" the star discrepancy we define $\delta$–covers as in [22]: for any $\delta \in (0,1]$ a finite set $\Gamma$ of points in $[0,1)^d$ is called a *$\delta$–cover* of $[0,1)^d$, if for every $y \in [0,1)^d$ there exist $x, z \in \Gamma \cup \{0\}$ such that $x \le y \le z$ and $\lambda^d([0,z]) - \lambda^d([0,x]) \le \delta$. The number $\mathcal{N}(d,\delta)$ denotes the smallest cardinality of a $\delta$–cover of $[0,1)^d$.

The following theorem was stated and proved in [37].

**Theorem 5.3.2.** *For any $d \ge 1$ and $\delta \in (0,1]$ we have*

$$\mathcal{N}(d,\delta) \le 2^d \frac{d^d}{d!}(\delta^{-1}+1)^d.$$

Notice that due to Stirling's formula we have $d^d/d! \le e^d/\sqrt{2\pi d}$ and so the cardinality of the $\delta-$cover may be bounded from above by $(2e)^d(1+\delta^{-1})^d$. Furthermore, it is easy to verify that in the case $d=1$ the identity

$$\mathcal{N}(1,\delta) = \lceil \delta^{-1} \rceil \tag{5.13}$$

is established with the help of the $\delta$-cover $\Gamma := \{1/\lceil\delta^{-1}\rceil, 2/\lceil\delta^{-1}\rceil, \dots, 1\}$.

With the help of $\delta$-covers the star discrepancy can be approximated in the following sense.

**Lemma 5.3.3.** *Let $P \subset [0,1)^d$ be an $N$-point set, $\delta > 0$, and $\Gamma$ be a $\delta$-cover of $[0,1)^d$. Then*

$$D_N^*(P) \le \max_{x\in\Gamma} D_N(P,x) + \delta.$$

The proof of Lemma 5.3.3 is straightforward, cf., e.g., [22, Lemma 3.1].

Now we are ready to prove Theorem 5.3.1.

*Proof of Theorem 5.3.1.* We will only prove the statement (5.12), the statement (5.11) follows then by easy calculations. For $\delta \in (0,1)$ to be chosen later let $\Gamma$ be a $\delta-$cover consisting of at most $(2e)^d(1+\delta^{-1})^d$ elements. Such a $\Gamma$ exists due to Theorem 5.3.2 and discussion thereafter.

Define

$$D_{N,\Gamma}^*(\mathcal{P}) = \max_{\beta\in\Gamma} \left| \lambda^d([0,\beta)) - \frac{1}{N}\sum_{j=1}^N \mathbf{1}_{[0,\beta)}(p_j) \right|.$$

Now Lemma 5.3.3 gives us

$$D_N^*(\mathcal{P}) \le D_{N,\Gamma}^*(\mathcal{P}) + \delta.$$

For every $\beta \in \Gamma$ and $j \in [N]$ put

$$\xi_\beta^{(j)} = \lambda^d([0,\beta)) - \mathbf{1}_{[0,\beta)}(p_j).$$

Let $\epsilon = 2\delta$. Due to Hoeffding's inequality applied to random variables $(\xi_\beta^{(j)})_{j=1}^N$ (applicable since $(p_j)_{j=1}^N$ is $e^{\rho d}$ - negatively dependent) we obtain for every $\beta \in \Gamma$

$$\mathbf{P}\left( \left| \frac{\sum_{j=1}^N \xi_\beta^{(j)}}{N} \right| \ge \delta \right) \le 2e^{\rho d} e^{-2N\delta^2}.$$

With the help of a simple union bound we get

$$\begin{aligned}
&\mathbf{P}(D_N^*(\mathcal{P}) < \epsilon) = 1 - \mathbf{P}(D_N^*(\mathcal{P}) \geq \epsilon) \\
&\geq 1 - \mathbf{P}(D_{N,\Gamma}^*(\mathcal{P}) \geq \epsilon - \delta) = 1 - \mathbf{P}\left(\max_{\beta\in\Gamma}\left|\frac{\sum_{j=1}^N \xi_\beta^{(j)}}{N}\right| \geq \delta\right) \\
&\geq 1 - 2e^{\rho d}|\Gamma|e^{-2N\delta^2}.
\end{aligned}$$

Using the above we would like to find a bound on discrepancy of the sampling scheme $\mathcal{P}$ which holds with probability at least $\theta \in (0,1)$. We are looking for $\epsilon_\theta$ such that

$$\mathbf{P}(D_N^*(\mathcal{P}) < \epsilon_\theta) \geq \theta. \tag{5.14}$$

Put $\epsilon_\theta = C_\theta(\frac{d}{N}\log(1+\frac{N}{d}))^{\frac{1}{2}} = 2\delta_\theta$. Inequality (5.14) holds true if

$$\delta_\theta \geq \left(\frac{1}{2N}\right)^{\frac{1}{2}}\left[\log(|\Gamma|) + \rho d + \log\left(\frac{2}{1-\theta}\right)\right]^{\frac{1}{2}}.$$

Our problem boils now down to finding possibly small $\delta_\theta \in (0,1)$ for which

$$\delta_\theta \geq \left(\frac{1}{2N}\right)^{\frac{1}{2}}\left[d\log\left(2e\left[1+\delta_\theta^{-1}\right]\right) + \rho d + \log\left(\frac{2}{1-\theta}\right)\right]^{\frac{1}{2}}. \tag{5.15}$$

Specifying $\delta_\theta$ to be of the form

$$\delta_\theta = \left(\frac{1}{2N}\right)^{\frac{1}{2}}\left[d\log(\eta) + \rho d + \log\left(\frac{2}{1-\theta}\right)\right]^{\frac{1}{2}}$$

we get that (5.15) is satisfied if

$$\eta \geq 2e\left(1+\delta_\theta^{-1}\right).$$

Expanding $\delta_\theta$ in dependence of $\eta$ it suffices to find $\eta$ for which

$$\left(\frac{\eta}{2e} - 1\right)\log(\eta)^{\frac{1}{2}} \geq \left(\frac{N}{2d}\right)^{\frac{1}{2}}$$

and one easily sees that this is satisfied for $\eta$ given in the statement of the theorem. □

### 5.3.2 Bound on the Weighted Star Discrepancy for $\mathcal{D}_0^d-\gamma$-negatively Dependent Sampling Schemes.

One of the reasons why the QMC integration may be successfully applied in many high-dimensional problems is the fact that quite often only a small number of coordinates is really important. This observation led to the introduction of weighted function spaces

and weighted discrepancies by Sloan and Woźniakowski in [103]. The above concepts are closely related to the theory of weighted spaces of Sobolev type, in particular the integration error in those spaces obeys a Koksma-Hlawka type upper bound, which may be phrased using the norm of the function and the weighted star discrepancy.

By weights we understand a set of non-negative numbers $\gamma = (\gamma_u)_{u\in[d]\setminus\emptyset}$, where $\gamma_u$ is interpreted as the weight of the coordinates from $u$. Let $|u|$ denote the cardinality of $u$. For $x \in [0,1]^d$ we write $(x(u),1)$ to denote the point in $[0,1]^d$ agreeing with $x$ on the coordinates from $u$ and having all the other coordinates set to 1.

The weighted star discrepancy of a point set $\mathcal{P} = (p_1,\dots,p_N)$ and weights $\gamma$ is defined by

$$D^*_{N,\gamma}(\mathcal{P}) := \sup_{z\in[0,1]^d} \max_{u\in[d]\setminus\emptyset} \gamma_u |D_N(\mathcal{P},(z(u),1)|.$$

The following theorem is similar in flavor to the Theorem 1 from [1].

**Theorem 5.3.4.** *Let $N,d \in \mathbb{N}$ and let $\mathcal{P} = (p_j)_{j=1}^N \subset [0,1)^d$ be a sampling scheme, such that for every $\emptyset \neq u \subset [d]$ its projection on the coordinates in $u$ is $\mathcal{D}_0^{|u|}$ - $e^{\rho|u|}$- negatively dependent. Then for any weights $(\gamma_u)_{u\subset[d]\setminus\emptyset}$ and any $c>0$ it holds*

$$D^*_{N,\gamma}(\mathcal{P}) \leq \max_{\emptyset\neq u\subset[d]} c\gamma_u \sqrt{\frac{|u|}{N}} \tag{5.16}$$

*with probability at least $2-(1+e^{-(1.6741c^2-10.7042-\rho)})^d$. Moreover, for $\theta\in(0,1)$ it holds*

$$\mathbf{P}\left( D^*_{N,\gamma}(\mathcal{P}) \leq \max_{\emptyset\neq u\subset[d]} \gamma_u \sqrt{\frac{|\rho+10.7042+\log((2-\theta)^{\frac{1}{d}}-1)|}{1.6741}} \sqrt{\frac{|u|}{N}} \right) \geq \theta. \tag{5.17}$$

*Proof.* We shall only prove the statement (5.16), the statement (5.17) follows then by simple calculations. For $\emptyset \neq u \subset [d]$ and $c>0$ put

$$A_u = \{\omega\in\Omega : D^*_N(\mathcal{P}^u(\omega)) > c\sqrt{\tfrac{|u|}{N}}\}.$$

Here $\mathcal{P}^u$ denotes the projection of $\mathcal{P}$ on the coordinates from $u$. By Theorem 5.2.9 it holds

$$\mathbf{P}(A_u) < e^{-(1.674c^2-10.7042-\rho)|u|}.$$

Now

$$\begin{aligned}
&\mathbf{P}\left( D^*_{N,\gamma}(\mathcal{P}) > \max_{\emptyset\neq u\subset[d]} c\gamma_u\sqrt{\frac{|u|}{N}} \right) \leq \mathbf{P}\Big( \bigcup_{\emptyset\neq u\subset[d]} A_u \Big) \\
&< \sum_{\nu=1}^{d} \binom{d}{\nu} e^{-(1.6741c^2-10.7042-\rho)\nu} \\
&= (1+e^{-(1.6741c^2-10.7042-\rho)})^d - 1.
\end{aligned}$$

□

## 5.4 Examples of Negatively Dependent and Pairwise Negatively Dependent Sampling Schemes

Many sampling schemes, such as randomly shifted and jittered rank-1 lattices and Latin hypercube sampling, are multidimensional generalizations of the one-dimensional simple stratified sampling.

**Definition 5.4.1.** Let $\pi$ be a uniformly chosen permutation of $\{1,\dots,N\}$ and let $(U_j)_{j=1}^N$ be independent random variables distributed uniformly on $(0,1]$. Moreover, $\pi$ is independent of $(U_j)_j$. We put

$$p_j := \frac{\pi(j) - U_j}{N}, j = 1,\dots,N.$$

The sampling scheme $\mathcal{P} = (p_j)_{j=1}^N$ is called *simple stratified sampling.*

Effectively, one is considering the partition $I_j := [\frac{j-1}{N}, \frac{j}{N}), j = 1,\dots,N$, of the unit interval and in every element of the partition putting one point, independently of all the other points. The straightforward observation that simple stratified sampling is pairwise negatively dependent is the starting point of our investigation.

Formally, at least for $N = b^m$, where $b \geq 2, m \geq 1$ are integers, pairwise negative dependence of stratified sampling may be deduced from [72]. Still, the proof presented there is rather involved, since it shall easily generalize to a proof of pairwise negative dependence of scrambled $(0,m,2)-$nets. For this reason we present here an easy argument yielding pairwise negative dependence of simple stratified sampling. Similar results may be also found in the literature, see e.g. Lemma 3.4. in [41].

**Lemma 5.4.2.** *Simple stratified sampling $\mathcal{P} = (p_j)_{j=1}^N$ is pairwise negatively dependent.*

*Proof.* Let $Q = [q,1), R = [r,1)$ be two boxes anchored at 1. Without loss of generality we may assume $R \subset Q$. We aim at showing

$$\mathbf{P}(p_1 \in Q | p_2 \in R) \leq \lambda(Q).$$

Let $\eta, \rho$ be such that $q \in I_\eta, r \in I_\rho$. Define $\epsilon_q := \eta - Nq, \epsilon_r := \rho - Nr$. We are considering two cases. In the first case $\eta < \rho$. Then it follows

$$\begin{aligned}
&\mathbf{P}(p_1 \in Q | p_2 \in R) = \mathbf{P}(p_1 \in Q, p_2 \in I_\rho | p_2 \in R) + \sum_{k=\rho+1}^{N} \mathbf{P}(p_1 \in Q, p_2 \in I_k | p_2 \in R) \\
&= \frac{N-\eta-1+\epsilon_q}{N} \frac{\epsilon_r}{N\lambda(R)} + \frac{N-\eta-1+\epsilon_q}{N} \frac{N-\rho}{N\lambda(R)} \\
&= \frac{N-\eta-1+\epsilon_q}{N} < \frac{N-\eta+\epsilon_q}{N} = \lambda(Q).
\end{aligned}$$

In the second case, $\eta = \rho$ and

$$\mathbf{P}(p_1 \in Q | p_2 \in R) = \mathbf{P}(p_1 \in Q, p_2 \in I_\eta | p_2 \in R) + \sum_{k=\eta+1}^{N} \mathbf{P}(p_1 \in Q, p_2 \in I_k | p_2 \in R)$$
$$= \frac{N-\eta}{N} \frac{\epsilon_r}{N\lambda(R)} + \frac{N-\eta-1+\epsilon_q}{N} \frac{N-\eta}{N\lambda(R)} < \frac{N-\eta+\epsilon_q}{N} = \lambda(Q).$$

□

Multidimensional extensions of simple stratified sampling include

a) stratified sampling in $[0,1)^d$, where the $N$ strata are axis parallel boxes,

b) Latin hypercube sampling,

c) randomly shifted and jittered rank-1 lattice,

c) scrambled $(t,m,d)-$nets in base $b \in \mathbb{N}_{\geq 2}$.

In this chapter we investigate the negative dependence properties of randomly shifted and jittered rank-1 lattices, Latin hypercube sampling and genralized stratified sampling. We describe known results on $(t,m,d)$-nets and show that concatenating negatively dependent sampling schemes one obtains negatively dependent sampling scheme in higher dimension.

### 5.4.1 Randomly Shifted and Jittered Rank-1 Lattice

Let $N$ be prime. We denote $\mathbb{F} := \mathbb{F}_N := \{0, 1, \ldots, N-1\}$. Moreover, $\mathbb{F}^* := \mathbb{F} \setminus \{0\}$. We also put $\widetilde{\mathbb{F}} := \frac{1}{N}\mathbb{F}$ and $\widetilde{\mathbb{F}}^* := \frac{1}{N}\mathbb{F}^*$.

A discrete subgroup $L$ of the $d-$dimensional torus $\mathbb{T}^d$ (where $\mathbb{T}^d = [0,1)^d$, the addition of two elements of $\mathbb{T}^d$ and the multiplication with reals is to be taken componentwise modulo 1.) is called a lattice.

**Definition 5.4.3.** A set $(y_j)_{j=1}^N \subset [0,1)^d$ is a *rank-1 lattice* if for some $g \in (\widetilde{\mathbb{F}}^*)^d$ it admits a representation

$$y_j = (j-1)g \bmod 1, \quad j = 1, \ldots, N.$$

In this case $g$ is called a generating vector of the lattice.

Note that, in particular, a rank-1 lattice is a cyclic subgroup of the torus.

We remark that our definition differs from the usual one in that we allow only for generating vectors $g$ from $(\widetilde{\mathbb{F}}^*)^d$ and not from $\widetilde{\mathbb{F}}^d$, which saves us from considering some degenerate cases.

We want now to define a sampling scheme based on rank-1 lattices.

**Definition 5.4.4.** Let $(y_j)_{j=1}^N$ be a rank-1 lattice with generating vector chosen uniformly at random from $(\widetilde{\mathbb{F}}^*)^d$. Let $S$ be distributed uniformly on $\widetilde{\mathbb{F}}^d$, $J_j, j = 1, \ldots, N$, be uniformly distributed on $[0, \frac{1}{N})^d$ and $\pi$ be a uniformly chosen permutation of $\{1, \ldots, N\}$. Moreover, let all of the aforementioned random variables be independent. We put

$$p_j := y_{\pi(j)} + S + J_j \bmod 1, \quad j = 1, \ldots, N.$$

The sampling scheme $\mathcal{P} = (p_j)_{j=1}^N$ is called a *randomly shifted and jittered rank-1 lattice (RSJ rank-1 lattice).*

Putting it in words: we first take a rank-1 lattice with a random generator and symmetrize it. Then we shift the lattice uniformly on the torus, where the shift has resolution $\frac{1}{N}$. In the last step we jitter every point independently of all the other points in a $d$-dimensional cube of volume $N^{-d}$.

### 5.4.2 Latin Hypercube Sampling

**Definition 5.4.5.** Let $(\pi_i)_{i=1}^d$ be independent uniformly chosen permutations of $\{1, \ldots, N\}$, and $U_j^{(i)}, i = 1, \ldots, d, j = 1, \ldots, N$, be independent random variables distributed uniformly on $(0, 1]$ and independent also of the permutations. A sampling scheme $(p_j)_{j=1}^N$ is called a *Latin hypercube sampling* if the $i-$th coordinate of the $j-$th point $p_j^{(i)}$ is given by

$$p_j^{(i)} = \frac{\pi_i(j) - U_j^{(i)}}{N}, \quad i = 1, \ldots, d, j = 1, \ldots, N. \tag{5.18}$$

What one intuitively does is the following: one cuts $[0, 1)^d$ into slices $(S_{k,j})_{j=1}^N, k = 1, \ldots, d$, given by

$$S_{k,j} = \prod_{j=1}^{k-1} [0, 1) \times [\tfrac{j-1}{N}, \tfrac{j}{N}) \times \prod_{j=k+1}^{d} [0, 1)$$

and places $N$ points in such a way that in every slice there is exactly one point.

Latin hypercube sampling was introduced in [76]. An earlier variant, known as lattice sampling, is due to [93]. There one simply substitutes the random variables $U_j^{(i)}$ in (5.18) by constant values $\frac{1}{2}$.

### 5.4.3 Pairwise Negative Dependence of RSJ Rank-1 Lattice and LHS

Our aim is now to show that RSJ rank-1 lattice is a coordinatewise independent NQD sampling scheme. In the course of the proof we will demonstrate that the bivariate copulas (in this case: cummulative distribution functions of a pair of points) of RSJ rank-1 lattice and LHS are the same.

Note that for $d = 1$ RSJ rank-1 lattice and LHS are nothing else but simple stratified sampling, the claim is therefore settled by Lemma 5.4.2.

Now we may turn our attention to the more interesting multidimensional case. Let $\mathcal{P} = (p_j)_{j=1}^N$ be a RSJ rank-1 lattice in $[0,1)^d, d \geq 2$. Put

$$D_d = \{(f_1, f_2) \in \mathbb{F}^d \times \mathbb{F}^d \mid f_1^{(i)} \neq f_2^{(i)}, i = 1, \ldots, d\},$$

and set $D := D_1$. A random variable $(p_1, p_2)$ having uniform distribution on pairs of distinct points from $\mathcal{P}$ may be generated in the following way: let $(m_1, m_2)$ be uniformly distributed on $D$ and let the random variables $g, S, J_1, \ldots, J_N$, be independent. The generating vector $g$ is distributed uniformly on $(\widetilde{\mathbb{F}}^*)^d$, the shift $S$ on $\widetilde{\mathbb{F}}^d$. If $J_j, j = 1, \ldots, N$, are almost surely all equal to 0, then we speak of the *discrete model*, and if $J_j, j = 1, \ldots, N$, are distributed uniformly on $[0, \frac{1}{N})^d$, we speak of the *continuous model*. Even though our aim is to investigate the continuous model, the discrete model will turn out to be helpful to highlight the combinatorial nature of the problem. Finally, we put for $j = 1, 2,\ i = 1, \ldots, d$,

$$p_j^{(i)} = (g^{(i)} m_j + S^{(i)}) \bmod 1 + J_j^{(i)}. \tag{5.19}$$

**Lemma 5.4.6.** *In the discrete model for $(z_1, z_2) \in \frac{1}{N} D_d$ and $(a, b) \in D$ it holds*

$$\mathbf{P}(p_1 = z_1, p_2 = z_2 | m_1 = a, m_2 = b) = \frac{1}{(N(N-1))^d}.$$

*In particular, in the discrete model*

$$\mathbf{P}(p_1 = z_1, p_2 = z_2) = \frac{1}{(N(N-1))^d}.$$

*Proof.* In the first step we show that for any $i = 1, \ldots, d$

$$\mathbf{P}(p_1^{(i)} = z_1^{(i)}, p_2^{(i)} = z_2^{(i)} | m_1 = a, m_2 = b) = \frac{1}{N(N-1)}. \tag{5.20}$$

It suffices to show that given $a, b, z_1^{(i)}, z_2^{(i)}$ the system of equations

$$\begin{cases} z_1^{(i)} = \gamma a + \nu & \bmod 1 \\ z_2^{(i)} = \gamma b + \nu & \bmod 1 \end{cases}$$

has exactly one solution $\gamma \in \widetilde{\mathbb{F}}^*, \nu \in \widetilde{\mathbb{F}}$. One solution is given by

$$\begin{cases} \gamma = (z_1^{(i)} - z_2^{(i)})(a-b)^{-1} \bmod 1 \\ \nu = (z_1^{(i)} - \gamma a) \bmod 1 \end{cases}$$

and it is indeed unique, since the determinant of the associated matrix is $(a-b) \neq 0 \bmod N$. Now we are ready to prove the claim of the theorem by induction on the dimension. Suppose the statement has already been proven for dimension $d$ and we want to prove

it for dimension $(d+1)$. For any $(d+1)-$dimensional (possibly random) vector $W$ we denote by $\widetilde{W}$ the projection onto its first $d$ coordinates. We have

$$\begin{aligned}&\mathbf{P}(p_1 = z_1, p_2 = z_2 | m_1 = a, m_2 = b)\\ &= \mathbf{P}(p_1^{(d+1)} = z_1^{(d+1)}, p_2^{(d+1)} = z_2^{(d+1)} | m_1 = a, m_2 = b, \widetilde{p}_1 = \widetilde{z}_1, \widetilde{p}_2 = \widetilde{z}_2)\\ &\times \mathbf{P}(\widetilde{p}_1 = \widetilde{z}_1, \widetilde{p}_2 = \widetilde{z}_2 | m_1 = a, m_2 = b).\end{aligned}$$

By induction assumption $\mathbf{P}(\widetilde{p}_1 = \widetilde{z}_1, \widetilde{p}_2 = \widetilde{z}_2 | m_1 = a, m_2 = b) = \frac{1}{(N(N-1))^d}$, hence it suffices to show

$$\mathbf{P}(p_1^{(d+1)} = z_1^{(d+1)}, p_2^{(d+1)} = z_2^{(d+1)} | m_1 = a, m_2 = b, \widetilde{p}_1 = \widetilde{z}_1, \widetilde{p}_2 = \widetilde{z}_2) = \frac{1}{N(N-1)}.$$

Note now that conditioned on $\{m_1 = a, m_2 = b\}$, the events $\{p_1^{(d+1)} = z_1^{(d+1)}, p_2^{(d+1)} = z_2^{(d+1)}\}$ and $\{\widetilde{p}_1 = \widetilde{z}_1, \widetilde{p}_2 = \widetilde{z}_2\}$ are independent and so we obtain

$$\begin{aligned}&\mathbf{P}(p_1^{(d+1)} = z_1^{(d+1)}, p_2^{(d+1)} = z_2^{(d+1)} | m_1 = a, m_2 = b, \tilde{p}_1 = \tilde{z}_1, \tilde{p}_2 = \tilde{z}_2)\\ &= \mathbf{P}(p_1^{(d+1)} = z_1^{(d+1)}, p_2^{(d+1)} = z_2^{(d+1)} | m_1 = a, m_2 = b) = \frac{1}{N(N-1)}.\end{aligned}$$

This proves the first statement. The second statement follows immediately by the law of total probability. □

**Corollary 5.4.7.** *(i) The random variables*

$$(p_1^{(i)}, p_2^{(i)}), \quad i = 1, \ldots, d,$$

*as defined in (5.19) are independent and identically distributed in the discrete as well as in the continuous model.*

*(ii) Randomly shifted and jittered rank-1 lattice has the same bivariate distributions as Latin hypercube sampling.*

*Proof.* To prove (i) note that for given $(z_1, z_2) \in \frac{1}{N} D_d$ we obtain from Lemma 5.4.6 applied to the one-dimensional case

$$\mathbf{P}(p_1^{(i)} = z_1^{(i)}, p_2^{(i)} = z_2^{(i)}) = \frac{1}{N(N-1)}, \quad i = 1, \ldots, d.$$

If $I \subset \{1, \ldots, d\}$, then by the same lemma applied to the $|I|-$dimensional case we see that

$$\mathbf{P}\left(\bigcap_{i \in I} \{p_1^{(i)} = z_1^{(i)}, p_2^{(i)} = z_2^{(i)}\}\right) = \frac{1}{(N(N-1))^{|I|}} = \prod_{i \in I} \mathbf{P}(p_1^{(i)} = z_1^{(i)}, p_2^{(i)} = z_2^{(i)}),$$

which yields the claim.

For (ii) let $(\widetilde{p}_j)_{j=1}^N$ be a LHS. Due to symmetrization $\widetilde{p}_1, \dots, \widetilde{p}_N$, are exchangeable and clearly we have that the random variables $(\widetilde{p}_1^{(i)}, \widetilde{p}_2^{(i)}), i = 1, \dots, d$, are independent. Furthermore, for arbitrary $(z_1, z_2) \in \frac{1}{N} D_d$ and a fixed $i \in \{1, \dots, d\}$ it holds

$$\mathbf{P}(\widetilde{p}_1^{(i)} \in [z_1^{(i)}, z_1^{(i)} + \tfrac{1}{N}), \widetilde{p}_2^{(i)} \in [z_2^{(i)}, z_2^{(i)} + \tfrac{1}{N})) = \frac{1}{N(N-1)}.$$

Since $\widetilde{p}_1, \dots, \widetilde{p}_N$, are also jittered independently in the intervals of volume $\frac{1}{N^d}$ the claim follows. □

**Remark 5.4.8.** Let $d \geq 2, N \geq 5$ be prime , $\mathcal{P} = (p_j)_{j=1}^N$ be a RSJ rank-1 lattice and $\widetilde{\mathcal{P}} = (\widetilde{p}_j)_{j=1}^N$ be a LHS in $[0,1)^d$. If $t \geq 3$, then the distributions of $(p_j)_{j=1}^t$ and $(\widetilde{p}_j)_{j=1}^t$ differ.

To see this consider the discrete model. We will show that given $a, b \in \frac{1}{N} D^d$ there exists exactly one point set $X$, consisting of $N$ points and corresponding to a RSJ rank-1 lattice such that $a, b \in X$, but there are $[(N-2)!]^{d-1}$ such point sets corresponding to LHS.

The statement about LHS is obvious, so we focus on the point set corresponding to RSJ rank-1 lattice. The existence of $X$ follows by taking the shift $a$ and the generating vector $(b-a) \bmod 1$. To see uniqueness recall that a rank-1 lattice is a cyclic subgroup of $\mathbb{T}^d$, therefore any difference of two distinct elements is a generator of the lattice and determines it uniquely. This means $(b-a) \bmod 1$ is a generator of the underlying lattice $L$ and $X = (L + a) \bmod 1$.

**Theorem 5.4.9.** *Let $\mathcal{P} = (p_j)_{j=1}^N$ be a RSJ rank-1 lattice (in that case let $N$ be prime) or a Latin hypercube sampling in $[0,1)^d$. Then $\mathcal{P}$ is a coordinatewise independent NQD sampling scheme. In particular, it is conditionally NQD and pairwise negatively dependent.*

*Proof.* That RSJ rank-1 lattice and LHS are coordinatewise independent NQD sampling schemes follows from Corollary 5.4.7 in conjunction with Lemma 5.4.2. The conditional NQD property follows in an obvious way. To see that $\mathcal{P}$ is also pairwise negatively dependent, put $Q = \prod_{i=1}^d [q^{(i)}, 1), R = \prod_{i=1}^d [r^{(i)}, 1)$. Due to Corollary 5.4.7 and Lemma 5.4.2

$$\mathbf{P}(p_1 \in Q, p_2 \in R) = \prod_{i=1}^d \mathbf{P}(p_1^{(i)} \in [q^{(i)}, 1), p_2^{(i)} \in [r^{(i)}, 1))$$

$$\leq \prod_{i=1}^s (1 - q^{(i)})(1 - r^{(i)}) \leq \mathbf{P}(p_1 \in Q)\, \mathbf{P}(p_2 \in R).$$

Theorems 5.4.9 and 5.2.7 imply the following Corollary.

**Corollary 5.4.10.** *Let $d, N \in \mathbb{N}$ and let $f : [0,1)^d \to \mathbb{R}$ be monotone in each coordinate and square-integrable. Denote by $\mu_{\mathcal{P}}$ a randomized QMC quadrature based on RSJ rank-1 lattice or LHS, using $N$ integration nodes and by $\mu^{MC}$ Monte Carlo quadrature using $N$ integration nodes. It holds*

$$\mathrm{Var}(\mu_{\mathcal{P}} f) \leq \mathrm{Var}(\mu^{MC} f).$$

*Proof.* The claim follows by 5.2.7 and the fact that RSJ rank-1 lattice and LHS are coordinatewise independent NQD sampling schemes. □

Negative dependence of Latin hypercube sample has been studied in [41]. Here we summarize the known results on the different notions of negative dependence of Latin hypercube sampling.

**Theorem 5.4.11.** *Latin hypercube Sample in* $[0,1)^d$ *is a sampling scheme which is*

*(i)* $\mathcal{D}_0^d$ *- e*$^d$ *- negatively dependent,*

*(ii)* $\mathcal{C}_0^d$ *- negatively dependent,*

### 5.4.4 Minimal Randomness for Randomly Shifted and Jittered Rank-1 Lattices

In this section let $d \geq 2$, and let $N \geq 5$ be a prime number. We want to argue that the randomization of rank-1 lattices proposed by us is in a way the minimal one leading to a pairwise negatively dependent sampling scheme. More precisely, we show that resigning from any step of the randomization (the random choice of the generating vector, the random uniform shift or the independent jittering) infringes either pairwise negative dependence or the sampling scheme property.

(i) First note that without the uniform shift we do not get a sampling scheme at all. Indeed, we have then $\mathbf{P}(p_1 \in [0, \frac{1}{N})^d) = \frac{1}{N}$.

(ii) Now consider a situation in which we just shift all the points of the rank-1 lattice (possibly generated by a random vector) by a uniformly chosen vector on the torus. Then obviously the distances between the points on the torus remain unchanged. Consider the distance function $\mathrm{dist} : [0,1)^2 \to [0,1)$ on the torus $\mathbb{T}^1$ given by

$$\mathrm{dist}(x,y) := \min\left(\max(x,y) - \min(x,y), 1 - \max(x,y) + \min(x,y)\right).$$

**Proposition 5.4.12.** *Let* $\mathcal{P} = (p_j)_{j=1}^N$ *be a sampling scheme such that for some* $i = 1, \ldots, d$*, there exist a constant* $0 < \epsilon \leq \frac{1}{2}$ *with*

$$\mathbf{P}(\mathrm{dist}(p_1^{(i)}, p_2^{(i)}) \leq \epsilon) = 0.$$

*Then* $\mathcal{P}$ *is not pairwise negatively dependent.*

*Proof.* Without loss of generality let $i = d$. Consider $Q := [0,1)^{d-1} \times [\frac{\epsilon}{2}, 1)$ and $R := [0,1)^{d-1} \times [1 - \frac{\epsilon}{2}, 1)$. We claim that

$$\mathbf{P}(p_1 \in Q | p_2 \in R) = 1, \tag{5.21}$$

which already implies the statement of the proposition. Let $p_2 \in R$. Since almost surely $\mathrm{dist}(p_1^{(d)}, p_2^{(d)}) > \epsilon$, we have $\mathbf{P}(p_1^{(d)} > \frac{\epsilon}{2} | p_2 \in R) = 1$ and so $\mathbf{P}(p_1 \in Q | p_2 \in R) = 1$. □

Proposition 5.4.12 shows that resigning from jittering we do not get a pairwise negatively dependent sampling scheme. As a side note, it also implies that lattice sampling, the earlier variant of LHS proposed by Patterson in [93], does not provide a pairwise negatively dependent sampling scheme.

(iii) Finally, consider the construction similar to the construction of RSJ rank-1 lattice, differing only in that we fix a generating vector. To see that there exists a generating vector for which it is not pairwise negatively dependent take $N = 5, g = (\frac{1}{5}, \frac{1}{5})$ and $Q = [\frac{3}{5}, 1)^2, R = [\frac{4}{5}, 1)^2$. Simple calculations reveal that in this case

$$\mathbf{P}(p_1 \in Q, p_2 \in R) = \tfrac{1}{5}\tfrac{1}{2\binom{5}{2}} = \tfrac{1}{100}$$

and

$$\mathbf{P}(p_1 \in Q)\,\mathbf{P}(p_2 \in R) = \tfrac{4}{625} < \tfrac{1}{100}.$$

### 5.4.5 Pairwise Negative Dependence of Scrambled (t,m,d)-Nets.

Let $t \in \mathbb{N}$. The so-called $(t, m, d)$-nets are genaralization of $(0, m, d)$-nets (see Definition 4.2.3) and belong to the most regular deterministic point sets. First defined by Niederreiter in [78], they have been subject of extensive research. For a nice introduction on $(t, m, d)$-nets and their randomization, see [75].

A $(t, m, d)$-*net* in base $b \in \mathbb{N}_{\geq 2}$ is any $P \subset [0, 1)^d$ such that for every elementary interval $E$ in base $b$ with $\lambda^d(E) = b^{-m+t}$ there are exactly $b^t$ point in $P \cap E$. It is easily seen that a $(t, m, d)$-net consists of exactly $b^{m+t}$ points. Specific constructions of $(t, m, d)$-nets are known.

Scrambling (see Section 4.2.1) a $(t, m, d)$-net results almost surely in a $(t, m, d)$-net.

In a recent article [73] J. Wiart and C. Lemieux have shown the following theorem (which follows from Corollary 4.10 from the aforementioned article)

**Theorem 5.4.13.** *Scrambled $(t, m, d)$-nets are pairwise negatively dependent sampling schemes if and only if $t = 0$.*

### 5.4.6 Negative Dependence of Generalized Stratified Sampling

We partition $[0, 1)^d$ into $\beta \geq N$ sets $(B_j)_{j=1}^{\beta}$ with $\lambda^d(B_j) = \frac{1}{\beta}, j = 1, \ldots, \beta$. Let $Y = (Y_1, \ldots, Y_\beta)$ be a random vector distributed uniformly on

$$\{(v_1, \ldots, v_\beta) \in \{0, 1\}^\beta : \sum_{j=1}^{\beta} v_j = N\}.$$

Given the value of $Y$ we place one point for each $j \in [\beta]$ with $Y_j = 1$ uniformly and independently of all other points inside $B_j$. Symmetrizing this construction yields a sampling scheme $\mathcal{P} = (p_j)_{j=1}^N$, which we call *generalized stratified sampling* (note that every single $p \in \mathcal{P}$ is uniformly distributed in $[0, 1)^d$). Here "generalized" has to be understood in the sense that there are possibly more strata then points.

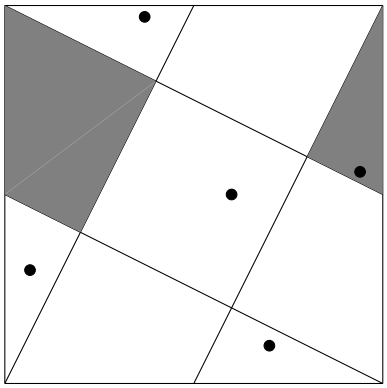

Figure 5.1: $N$ elementary cells of a rank-1 lattice as strata, $\beta = N = 5$.

**Example 5.4.14.** *There are many natural choices for the strata. The simplest one would be stripes of the form $B_j, j = 1, \dots, N$, with $B_j := [\frac{j-1}{N}, \frac{j}{N}) \times [0,1)^{d-1}$. Alternatively, one may divide $[0,1)^d$ into $N = n^d$ cubes of equal size. However, one could also choose, e.g., elementary cells (i.e., fundamental parallelepipeds) of a rank-1 lattice (cf. [69]), see Figure 5.1.*

To show that generalized stratified sampling is negatively dependent we need first a simple lemma.

**Lemma 5.4.15.** *Let $t, N \in \mathbb{N}, t \leq N, \xi \geq 0$ and let*

$$D = \{x = (x_1, \dots, x_N) \in \mathbb{R}^N \mid x \geq 0, \sum_{i=1}^{N} x_i = \xi\}.$$

*The function*

$$f : D \to \mathbb{R}, (x_1, \dots, x_N) \mapsto \sum_{J \subset [N], |J| = t} \prod_{j \in J} x_j$$

*takes on its maximum in the point $z = (z_1, \dots, z_N) = (\frac{\xi}{N} \dots, \frac{\xi}{N})$ and $f(z) = \binom{N}{t} \left(\frac{\xi}{N}\right)^t$.*

*Proof.* We shall prove the statement by induction on $N \geq t$. The case $N = t$ is straightforward by Lagrange multipliers theorem. Suppose we have already shown the statement for $N - 1$ and we would like to prove it for $N$. Firstly let us fix the value of $x_N \in (0, \xi)$. It holds

$$\begin{aligned} \sum_{J \subset [N], |J| = t} \prod_{j \in J} x_j &= \sum_{J \subset [N], |J| = t, N \in J} \prod_{j \in J} x_j + \sum_{J \subset [N], |J| = t, N \notin J} \prod_{j \in J} x_j \\ &= x_N \sum_{J' \subset [N-1], |J'| = t-1} \prod_{j \in J'} x_j + \sum_{J' \subset [N-1], |J'| = t} \prod_{j \in J'} x_j. \end{aligned}$$

By the induction assumption for a fixed value of $x_N$ the last term is maximal when for $j = 1, \dots, N-1$ we have $x_j = \frac{\eta}{N-1}$, where we put $\eta = \xi - x_N$. Plugging it into the above

formula we obtain

$$\sum_{J\subset[N],|J|=t}\prod_{j\in J}x_j=(\xi-\eta)\binom{N-1}{t-1}\left(\frac{\eta}{N-1}\right)^{t-1}+\binom{N-1}{t}\left(\frac{\eta}{N-1}\right)^{t},$$

which we need to maximize with respect to $\eta$. It holds

$$\sum_{J\subset[N],|J|=t}\prod_{j\in J}x_j=Ch(\eta),$$

where $C=\frac{(N-1)!}{(t-1)!(N-t)!(N-1)^{t-1}}$ and $h(\eta)=\xi\eta^{t-1}+\left(\frac{N-t}{t(N-1)}-1\right)\eta^t$. Now we have

$$h'(\eta)=\eta^{t-2}\left[(t-1)\xi+\left(\frac{N-t}{N-1}-t\right)\eta\right].$$

The derivative vanishes for $t\geq 3$ at $\eta_1=0$ and $\eta_2=\frac{N-1}{N}\xi$. Since $h(\eta_2)>\max\{h(0),h(\xi)\}$ and $\eta_2$ is a local maximum the claim follows. □

**Theorem 5.4.16.** *Let $\mathcal{P}=(p_j)_{j=1}^N$ be a generalized stratified sampling as described above and $A\subset[0,1)^d$ be measurable. Then for every $1\leq t\leq N$ it holds*

$$\mathbf{P}(\bigcap_{j=1}^{t}\{p_j\in A\})\leq\prod_{j=1}^{t}\mathbf{P}(p_j\in A).$$

*In particular, generalized stratified sampling is $\mathcal{S}$ - negatively dependent for any system $\mathcal{S}$ of measurable subsets of $[0,1)^d$.*

*Proof.* Fix $t$ as in the statement of the theorem and define

$$V_t=\{(k_1,\dots,k_t)\in[\beta]^t:\forall_{i,j\in[t]}\ \ i\neq j\implies k_i\neq k_j\}.$$

Note that $|V_t|=\beta(\beta-1)\cdots(\beta-t+1)$. For $k=(k_1,\dots,k_t)\in V_t$ we have

$$\mathbf{P}(\bigcap_{j=1}^{t}\{Y_{k_j}=1\})=\frac{\binom{\beta-t}{N-t}}{\binom{\beta}{N}}=\frac{N(N-1)\cdots(N-t+1)}{\beta(\beta-1)\cdots(\beta-t+1)}.$$

By Lemma 5.4.15 it follows

$$
\begin{aligned}
&\mathbf{P}(\bigcap_{j=1}^{t}\{p_j \in A\}) \\
&= \sum_{k\in V_t} \mathbf{P}(\bigcap_{j=1}^{t}\{p_j \in A\}|\bigcap_{j=1}^{t}\{p_j \in B_{k_j}\})\,\mathbf{P}(\bigcap_{j=1}^{t}\{p_j \in B_{k_j}\}|\bigcap_{j=1}^{t}\{Y_{k_j}=1\})\,\mathbf{P}(\bigcap_{j=1}^{t}\{Y_{k_j}=1\}) \\
&= \sum_{k\in V_t}\prod_{j=1}^{t}\frac{\lambda^d(A\cap B_{k_j})}{\lambda^d(B_{k_j})}\frac{1}{N(N-1)\cdots(N-t+1)}\frac{N(N-1)\cdots(N-t+1)}{\beta(\beta-1)\cdots(\beta-t+1)} \\
&= \frac{1}{\beta(\beta-1)\cdots(\beta-t+1)}\sum_{k\in V_t}\prod_{j=1}^{t}\frac{\lambda^d(A\cap B_{k_j})}{\lambda^d(B_{k_j})} \\
&\leq \frac{1}{\beta(\beta-1)\cdots(\beta-t+1)}\beta(\beta-1)\cdots(\beta-t+1)\left(\frac{\lambda^d(A)}{\beta}\right)^t\beta^t = (\lambda^d(A))^t.
\end{aligned}
$$

□

**Remark 5.4.17.** Without further information on the strata we cannot make any conclusions about pairwise negative dependence of generalized stratified sampling. As an example consider a stratified sampling scheme $\mathcal{P} = (p_1, p_2)$ defined by two strata $B_1, B_2$ in $d \geq 2$. One may choose $B_1, B_2$ and $Q, R \in \mathcal{C}_1^d$ in such a way that $Q \subset B_1, B_2 \subset R$ and $R \neq [0,1)^d$, see Figure 5.2. In this case however

$$\mathbf{P}(p_2 \in R | p_1 \in Q) = 1,$$

and the sampling scheme is not pairwise negatively dependent.

On the other hand if we consider strata $B_j, j = 1, \ldots, N$, with $B_j := [\frac{j-1}{N}, \frac{j}{N}) \times [0,1)^{d-1}$ then this practically boils down to the one-dimensional case and so the corresponding sampling scheme is pairwise negatively dependent, cf. Lemma 5.4.2.

### 5.4.7 Mixed Randomized Sequences

As already mentioned, part of the success of RQMC stems from the fact that in many high-dimensional practical integration problems only a small number of coordinates is of real importance. It stands to reason that one tries to use it to his avail by constructing quadratures in which one uses RQMC on the "important" coordinates and simple (usually much cheaper) Monte Carlo for the rest of the coordinates. This method is sometimes referred to as padding and the resulting sequences of integration nodes are called hybrid - Monte Carlo sequences. Let us give a formal definition.

**Definition 5.4.18.** Let $d, d', d'' \in \mathbb{N}$ with $d = d' + d''$. Let $X = (X_k)_{k\in\mathbb{N}}$ be a sequence in $[0,1)^{d'}$, and let $Y = (Y_k)_{k\in\mathbb{N}}$ be a sequence in $[0,1)^{d''}$. The $d$-dimensional concatenated sequence $Z = (Z_k)_{k\in\mathbb{N}} = (X_k, Y_k)_{k\in\mathbb{N}}$ is called a *mixed sequence*. If $Y$ is a sequence of

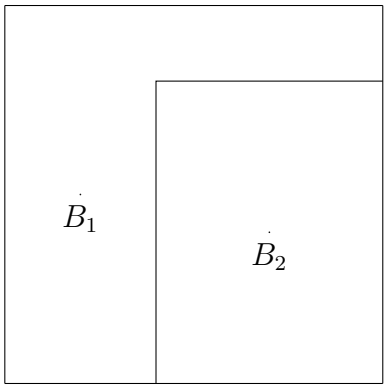


Figure 5.2: Example of strata for Remark 5.4.17

independent uniformly distributed random points, one also says that $Z$ results from $X$ by *padding by Monte Carlo* and calls $Z$ a *hybrid-Monte Carlo sequence*. If $X$ and $Y$ are both randomized sequences, we call $Z$ a *mixed randomized sequence*.

The definition carries over in a natural way to the case when $X$ and $Y$ are finite point sets with the same cardinality.

Padding by Monte Carlo was introduced by Spanier in [105] to tackle problems in particle transport theory. He suggested to use a hybrid-Monte Carlo sequence resulting from padding a deterministic low-discrepancy sequence. Hybrid-Monte Carlo sequences showed a favorable performance in several numerical experiments, see, e.g., [87, 88]. The latter papers also provided theoretical results on probabilistic discrepancy estimates of hybrid-Monte Carlo sequences which have been improved in [3, 38]. Favorable discrepancy bounds for padding Latin hypercube sampling (LHS) by Monte Carlo were provided in [41]. Padding a sequence by LHS (instead of by Monte Carlo) was considered earlier by Owen [89, Example 5].

A related line of research, initiated in [80], is to study the discrepancy of concatenated sequences that result from two deterministic sequences. More recent results can, e.g., be found in [47, 23, 62] and the literature mentioned therein.

The following proposition shows that concatenating two mutually independent negatively dependent sampling schemes results again in a (higher dimensional) negatively dependent sampling scheme. A weaker version of the next proposition may be found in [53]; cf. Lemma 5 there.

**Proposition 5.4.19.** *Let $d, d', d'' \in \mathbb{N}$ such that $d = d' + d''$. Let $A \subseteq [0,1)^{d'}$, $B \subseteq [0,1)^{d''}$ be Borel measurable sets. Let $x_1, \dots, x_N$ be a sampling scheme in $[0,1)^{d'}$ and $y_1, \dots, y_N$ a sampling scheme in $[0,1)^{d''}$. Furthermore, let $\alpha, \beta \geq 1$.*

*(i) If the random variables $\mathbf{1}_A(x_i)$, $i = 1, \dots, N$, and $\mathbf{1}_B(y_i)$, $i = 1, \dots, N$, are upper negatively $\alpha$- and $\beta$-dependent, respectively, and mutually independent, then the random variables $\mathbf{1}_{A\times B}(x_i, y_i)$, $i = 1, \dots, N$, induced by the random vectors $(x_1, y_1), \dots, (x_N, y_N)$ in $[0,1)^d$, are upper negatively $\alpha\beta$-dependent.*

*(ii) If the random variables $\mathbf{1}_A(x_i)$, $i = 1, \ldots, N$, and $\mathbf{1}_B(y_i)$, $i = 1, \ldots, N$, are lower negatively $\alpha$- and $\beta$-dependent, respectively, and mutually independent, then the random variables $\mathbf{1}_{A\times B}(x_i, y_i)$, $i = 1, \ldots, N$, induced by the random vectors $(x_1, y_1)$, ... ,$(x_N, y_N)$ in $[0,1)^d$, are lower negatively $\alpha\beta$-dependent.*

*Proof.* Let us first prove statement (i). Obviously for $J \subseteq [N]$ we have

$$\begin{aligned}
&\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}(x_j, y_j) = 1\}\right) = \mathbf{P}\left(\bigcap_{j\in J}\{x_j \in A\} \cap \bigcap_{j\in J}\{y_j \in B\}\right) \\
&= \mathbf{P}\left(\bigcap_{j\in J}\{x_j \in A\}\right)\mathbf{P}\left(\bigcap_{j\in J}\{y_j \in B\}\right) \leq \left(\alpha\prod_{j\in J}\mathbf{P}(x_j \in A)\right)\left(\beta\prod_{j\in J}\mathbf{P}(y_j \in B)\right) \\
&= \alpha\beta\prod_{j\in J}\mathbf{P}\left(\mathbf{1}_{A\times B}(x_j, y_j) = 1\right).
\end{aligned}$$

We now prove statement (ii). Take any $\emptyset \neq J \subseteq [N]$ and set $t = |J|$ . Suppose first that $((x_j, y_j))_{j=1}^N$ is a hybrid-Monte Carlo sequence, i.e., $(y_j)_{j=1}^N$ is a Monte Carlo sampling scheme. Due to our assumptions in statement (ii) we obtain

$$\begin{aligned}
&\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}(x_j, y_j) = 0\}\right) \\
&= \sum_{K\subseteq J}\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}(x_j, y_j) = 0\} \cap \bigcap_{j\in K}\{\mathbf{1}_B(y_j) = 1\} \cap \bigcap_{j\in J\setminus K}\{\mathbf{1}_B(y_j) = 0\}\right) \\
&= \sum_{\nu=0}^{t}\binom{t}{\nu}\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_A(x_j) = 0\}\right)\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_B(y_j) = 1\} \cap \bigcap_{j=\nu+1}^{t}\{\mathbf{1}_B(y_j) = 0\}\right) \\
&\leq \alpha\sum_{\nu=0}^{t}\binom{t}{\nu}\mathbf{P}\left(\mathbf{1}_A(x_1) = 0\right)^{\nu}\mathbf{P}\left(1_B(y_1) = 1\right)^{\nu}\mathbf{P}\left(\mathbf{1}_B(y_1) = 0\right)^{t-\nu} \\
&= \alpha[\mathbf{P}(\mathbf{1}_A(x_1) = 0)\,\mathbf{P}(\mathbf{1}_B(y_1) = 1) + \mathbf{P}(\mathbf{1}_B(y_1) = 0)]^t = \alpha\,\mathbf{P}(\mathbf{1}_{A\times B}(x_1, y_1) = 0)^t.
\end{aligned}$$

Now let $(y_j)_{j=1}^N$ be any sampling scheme in $[0,1)^{d''}$ such that the random variables $(\mathbf{1}_B(y_j))_{j=1}^N$ are lower $\beta$-negatively dependent and let $(\hat{y}_j)_{j=1}^N$ be a Monte Carlo sampling scheme in $[0,1)^{d''}$; we assume both sampling schemes to be mutually independent to $(x_j)_{j=1}^N$. Anal-

ogously as in the previous case we obtain

$$\begin{aligned}
&\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}(x_j,y_j)=0\}\right)\\
&=\sum_{\nu=0}^{t}\binom{t}{\nu}\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_A(x_j)=1\}\cap\bigcap_{j=\nu+1}^{t}\{\mathbf{1}_A(x_j)=0\}\right)\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_B(y_j)=0\}\right)\\
&\leq\sum_{\nu=0}^{t}\binom{t}{\nu}\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_A(x_j)=1\}\cap\bigcap_{j=\nu+1}^{t}\{\mathbf{1}_A(x_j)=0\}\right)\beta\,\mathbf{P}\left(\mathbf{1}_B(y_1)=0\right)^{\nu}\\
&=\beta\sum_{\nu=0}^{t}\binom{t}{\nu}\mathbf{P}\left(\bigcap_{j=1}^{\nu}\{\mathbf{1}_A(x_j)=1\}\cap\bigcap_{j=\nu+1}^{t}\{\mathbf{1}_A(x_j)=0\}\right)\mathbf{P}\left(\mathbf{1}_B(\hat{y}_1)=0\right)^{\nu}.
\end{aligned}$$

It follows from the case of hybrid-Monte Carlo sequences that

$$\begin{aligned}
&\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}(x_j,y_j)=0\}\right)\leq\beta\,\mathbf{P}\left(\bigcap_{j\in J}\{\mathbf{1}_{A\times B}\}(x_j,\hat{y}_j)=0\}\right)\\
&\leq\alpha\beta\,\mathbf{P}\left(\mathbf{1}_{A\times B}(x_1,\hat{y}_1)=0\right)^t=\alpha\beta\,\mathbf{P}\left(\mathbf{1}_{A\times B}(x_1,y_1)=0\right)^t
\end{aligned}$$

□

**Remark 5.4.20.** It follows easily on closer examination of the proof that for the statement (i) of Proposition 5.4.19 to hold true we need only $(\mathbf{1}_A(x_j))_{j=1}^N$ and $(\mathbf{1}_B(y_j))_{j=1}^N$ to be negatively $\alpha$- respectively $\beta$-upper dependent point sets, not necessarily sampling schemes. Moreover, if in (ii) we assume that $(y_j)_{j=1}^N$ is a Monte Carlo sampling scheme we also do not need to assume that $(x_j)_{j=1}^N$ is a sampling scheme.

**Remark 5.4.21.** Let $\mathcal{S}'$, $\mathcal{S}''$ be systems of measurable sets in $[0,1)^{d'}$ and $[0,1)^{d''}$, respectively. Let $(x_j)_{j=1}^N$ be an $\mathcal{S}'$-$\alpha$-negative dependent sampling scheme in $[0,1)^{d'}$ and $(y_j)_{j=1}^N$ an $\mathcal{S}''$-$\beta$-negative dependent sampling scheme in $[0,1)^{d''}$; both sampling schemes should be mutually independent. Furthermore, let $\mathcal{P}:=(p_j)_{j=1}^N$ be the resulting concatenated sampling scheme in $[0,1)^d$, i.e., $p_i:=(x_i,y_i)$, $i=1,\dots,N$.

(i) If $\mathcal{S}'=\mathcal{C}_0^{d'}$ and $\mathcal{S}''=\mathcal{C}_0^{d''}$, we obtain from Proposition 5.4.19 that the mixed randomized sequence $(p_j)_{j=1}^N$ is $\mathcal{C}_0^d$-$\alpha\beta$-negatively dependent, which implies that we may directly apply Theorem 5.3.1 to obtain a probabilistic discrepancy bound for $\mathcal{P}$.

(ii) If $\mathcal{S}'=\mathcal{D}_0^{d'}$ and $\mathcal{S}''=\mathcal{D}_0^{d''}$, we obtain from Proposition 5.4.19 that $(p_j)_{j=1}^N$ is $\alpha\beta$-negatively dependent with respect to the set system

$$\mathcal{D}_0^{d'}\times\mathcal{D}_0^{d''}:=\{D'\times D''\,|\,D'\in\mathcal{D}_0^{d'},D''\in\mathcal{D}_0^{d''}\}\neq\mathcal{D}_0^d.$$

Hence Theorem 5.2.9 is unfortunately not directly applicable to $\mathcal{P}$. Nevertheless, one may prove a counterpart of Theorem 5.2.9 with slightly worse constants that

relies on negative dependence with respect to $\mathcal{D}_0^{d'} \times \mathcal{D}_0^{d''}$. Namely, one may show for every $\theta \in (0,1)$ that

$$\mathbf{P}\left( D_N^*(\mathcal{P}) \leq 2 * 0.7729 \sqrt{10.7042 + \rho + \frac{\ln\left((1-\theta)^{-1}\right)}{d}} \sqrt{\frac{d}{N}} \right) \geq \theta. \tag{5.22}$$

The bound is based on the following simple observation: To estimate the local discrepancy of $\mathcal{P}$ in a test box $Q \in \mathcal{C}_0^d$, the strategy used in [41] (and earlier in [2]) is to decompose $Q$ into finitely many disjoint differences of boxes $\Delta_1, \ldots, \Delta_K \in \mathcal{D}_0^d$ such that $Q = \cup_{\nu=1}^K \Delta_\nu$. This gives

$$D_N(\mathcal{P}, Q) \leq \sum_{\nu=1}^K D_N(\mathcal{P}, \Delta_\nu). \tag{5.23}$$

By a mild abuse of notation, for a set $S \subseteq [0,1)^d$ we denote here $D_N(\mathcal{P}, S) = \left| \frac{|\mathcal{P} \cap S|}{N} - \lambda^d(S) \right|$. Now let us consider a fixed index $\nu$. Then we find $A_\nu, B_\nu \in \mathcal{C}_0^d$ such that $A_\nu \subseteq B_\nu$ and $\Delta_\nu = B_\nu \setminus A_\nu$. Furthermore, we may write $A_\nu = A'_\nu \times A''_\nu$ and $B_\nu = B'_\nu \times B''_\nu$ with $A'_\nu, B'_\nu \in \mathcal{C}_0^{d'}$ and $A''_\nu, B''_\nu \in \mathcal{C}_0^{d''}$. Then we may represent $\Delta_\nu$ as disjoint union

$$\Delta_\nu = (B'_\nu \setminus A'_\nu) \times B''_\nu \cup A'_\nu \times (B''_\nu \setminus A''_\nu) =: C_\nu^1 \cup C_\nu^2.$$

Thus

$$D_N(\mathcal{P}, \Delta_\nu) \leq D_N(\mathcal{P}, C_\nu^1) + D_N(\mathcal{P}, C_\nu^2), \tag{5.24}$$

where $C_\nu^1, C_\nu^2 \in \mathcal{D}_0^{d'} \times \mathcal{D}_0^{d''}$. Now large deviation inequalities of Bernstein- and Hoeffding-type can be used to obtain for each of the random variables $D_N(\mathcal{P}, C_\nu^1)$, $D_N(\mathcal{P}, C_\nu^2)$ the same upper bound as for the local discrepancy $D_N(\mathcal{P}^*, \Delta_\nu)$ of a $\mathcal{D}_0^d$-$\alpha\beta$-negative dependent sampling scheme $\mathcal{P}^*$ in the proof of [41, Theorem 4.3]. This, combined with (5.23) und (5.24), results in a probabilistic discrepancy bound for $D_N^*(\mathcal{P})$ that is as most as twice as big as the one from Theorem 5.2.9; for further details see [41, Proof of Theorem 4.3].

## 5.5 Relations Between Notions of Negative Dependence

It may be easily seen that the coordinatewise independent NQD property implies the pairwise negative dependence property as well as the conditional NQD property. It turns out that this is the only valid implication between the considered notions of negative dependence. In this section we give examples showing that other implications do not hold.

### 5.5.1 Pairwise Negative Dependence and Negative Dependence

Neither the pairwise negative dependence of a sampling scheme implies the negative dependence, nor the other way round.

**Example 5.5.1.** *We first show an example of a negatively dependent sampling scheme which is neither pairwise negatively dependent nor conditionally NQD. To this end consider a sampling scheme consisting of just two points $\mathcal{P} = (p_1, p_2)$ in $[0, 1)$ with joint CDF $F : [0, 1]^2 \to [0, 1]$ given by*

$$F(x, y) = \min\{x, y, \tfrac{x^2+y^2}{2}\}.$$

*It is easy to see that $F(0, 0) = 0, F(1, 1) = 1, F$ is continuous, quasimonotone, and $F(x, y) = F(y, x)$, which implies that $F$ is a CDF of a sampling scheme. Moreover,*

$$\mathbf{P}\left(p_1 \in [0, q), p_2 \in [0, q)\right) = F(q, q) = q^2,$$

*so the sampling scheme is $\mathcal{C}_0^1$ - negatively dependent. Notice that due to $d = 1$, it is equivalent to saying that the sampling scheme is $\mathcal{C}_1^1$ - negatively dependent. However, for instance*

$$\begin{aligned}&\mathbf{P}(p_1 \in [\tfrac{3}{4}, 1), p_2 \in [\tfrac{1}{4}, 1)) = 1 - (F(\tfrac{3}{4}, 1) + F(1, \tfrac{1}{4}) - F(\tfrac{3}{4}, \tfrac{1}{4}))\\ &= F(\tfrac{3}{4}, \tfrac{1}{4}) = \tfrac{1}{4} > (1 - \tfrac{3}{4})(1 - \tfrac{1}{4}) = \mathbf{P}(p_1 \in [\tfrac{3}{4}, 1))\,\mathbf{P}(p_2 \in [\tfrac{1}{4}, 1)).\end{aligned}$$

*Notice that for $d = 1$ the notions of pairwise negatively dependent sampling scheme and conditionally NQD sampling scheme coincide.*

**Example 5.5.2.** *To see that even the stronger coordinatewise independent NQD property does not imply the negative dependence property consider RSJ rank-1 lattice $(p_j)_{j=1}^N$, defined in Subsection 5.4.1. On the one hand, according to Theorem 5.4.9, RSJ rank-1 lattice is coordinatewise independent NQD. On the other hand, let us consider the situation for $d = 2$, and a large $N$ to be chosen later. We put $Q = [0, \frac{3}{N})^2$. Obviously*

$$\mathbf{P}(p_1 \in Q)^3 = \left(\frac{3}{N}\right)^6.$$

*We also have*

$$\mathbf{P}(p_1 \in Q, p_2 \in Q, p_3 \in Q) \geq \frac{1}{\binom{N}{3} N(N-1)} = \frac{6}{N^2(N-1)^2(N-2)},$$

*the inequality follows since for the diagonal configuration of the points (i.e. $p_j = (\frac{\pi(j)}{N}, \frac{\pi(j)}{N}) + J_j, j = 1, \ldots, n$ for some permutation $\pi$ of $\{1, \ldots, N\}$) there is one triple of points always lying in $Q$. Notice that any generating vector of the form $g = (\frac{k}{N}, \frac{k}{N}), k \in [N-1]$ and any shift of the form $S = (\frac{l}{N}, \frac{l}{N}), l \in \{0, 1, \ldots, N-1\}$, results in a diagonal configuration. Now for $N$ large enough it holds*

$$\mathbf{P}(p_1 \in Q, p_2 \in Q, p_3 \in Q) > \mathbf{P}(p_1 \in Q)^3.$$

### 5.5.2 Conditional NQD and Pairwise Negative Dependence

**Example 5.5.3.** *First we show an example of a pairwise negatively dependent sampling scheme which is not conditionally NQD. Let* $B_1 = [0, \frac{1}{2})^2, B_2 = [\frac{1}{2}, 1) \times [0, \frac{1}{2}), B_3 = [0, \frac{1}{2}) \times [\frac{1}{2}, 1), B_4 = [\frac{1}{2}, 1)^2$ *denote the slots. Now we are considering a sampling scheme* $\mathcal{P} = (p_1, p_2)$ *such that given the slots the points are distributed uniformly within the slots and are independent. Denote* $A_{ij} := \{p_1 \in B_i, p_2 \in B_j\}$ *and set*

$$\mathbf{P}(A_{ii}) = \tfrac{1}{16}, i = 1, 2, 3, 4,$$

$$\mathbf{P}(A_{13}) = \mathbf{P}(A_{24}) = \mathbf{P}(A_{31}) = \mathbf{P}(A_{42}) = \tfrac{1}{32},$$
$$\mathbf{P}(A_{14}) = \mathbf{P}(A_{23}) = \mathbf{P}(A_{41}) = \mathbf{P}(A_{32}) = \tfrac{5}{32}.$$

*It is easy to see that* $\mathcal{P}$ *is not conditionally NQD, e.g.*

$$\begin{aligned}&\mathbf{P}(p_1^{(2)} \geq \tfrac{1}{2}, p_2^{(2)} \geq \tfrac{1}{2} | p_1^{(1)} \geq \tfrac{1}{2}, p_2^{(1)} \geq \tfrac{1}{2}) = \tfrac{1}{3}\\ &> \tfrac{1}{4} = \mathbf{P}(p_1^{(2)} \geq \tfrac{1}{2} | p_1^{(1)} \geq \tfrac{1}{2}, p_2^{(1)} \geq \tfrac{1}{2})\, \mathbf{P}(p_2^{(2)} \geq \tfrac{1}{2} | p_1^{(1)} \geq \tfrac{1}{2}, p_2^{(1)} \geq \tfrac{1}{2}).\end{aligned}$$

*Showing that* $\mathcal{P}$ *is pairwise negatively dependent requires simple but tedious calculations and as such will be omitted. Intuitively it is clear, since the sampling scheme gives high probability to diagonal arrangements (i.e.* $A_{14}, A_{23}, A_{41}, A_{32}$*).*

**Example 5.5.4.** *Now we show an example of a sampling scheme which is conditionally NQD but not pairwise negatively dependentd. To this end let* $X, Y$ *be two independent random variables distributed uniformly on* $[0, 1)$*. We consider a sampling scheme* $\mathcal{P} = (p_1, p_2)$ *given by* $p_1 = (X, Y), p_2 = (Y, X)$*. Let* $u, v \in [0, 1)^2$ *and* $A, B \subset [0, 1)$ *be measurable. Sampling scheme* $\mathcal{P}$ *is conditionally NQD since*

$$\begin{aligned}&\mathbf{P}(p_1^{(2)} \geq u^{(2)}, p_2^{(2)} \geq v^{(2)} | p_1^{(1)} \in A, p_2^{(1)} \in B)\\ &= \mathbf{P}(Y \geq u^{(2)}, X \geq v^{(2)} | X \in A, Y \in B)\\ &= \mathbf{P}(Y \geq u^{(2)} | X \in A, Y \in B)\, \mathbf{P}(X \geq v^{(2)} | X \in A, Y \in B)\\ &= \mathbf{P}(p_1^{(2)} \geq u^{(2)} | X \in A, Y \in B)\, \mathbf{P}(p_2^{(2)} \geq v^{(2)} | X \in A, Y \in B).\end{aligned}$$

*On the other hand* $\mathcal{P}$ *is not pairwise negatively dependent. To see this note that*

$$\begin{aligned}&\mathbf{P}(p_1 \geq u)\, \mathbf{P}(p_2 \geq v)\\ &= \mathbf{P}(X \geq u^{(1)}, Y \geq u^{(2)})\, \mathbf{P}(Y \geq v^{(1)}, X \geq v^2)\\ &= \mathbf{P}(X \geq u^{(1)})\, \mathbf{P}(Y \geq u^{(2)})\, \mathbf{P}(Y \geq v^{(1)})\, \mathbf{P}(X \geq v^{(2)})\end{aligned}$$

*and*

$$\mathbf{P}(p_1 \geq u, p_2 \geq v) = \mathbf{P}(X \geq \max(u^{(1)}, v^{(2)}), Y \geq \max(u^{(2)}, v^{(1)})).$$

*Taking for some* $u^{(1)}, u^{(2)} \in (0, 1)$ *the point* $v$ *satisfying* $v^{(1)} = u^{(2)}$ *and* $v^{(2)} = u^{(1)}$ *yields the claim.*

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