Quasi-Monte Carlo methods for high-dimensional integration – the standard (weighted Hilbert space) setting and beyond

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Abstract

This paper is a contemporary review of QMC ("quasi-Monte Carlo") methods, i.e., equal-weight rules for the approximate evaluation of high-dimensional integrals over the unit cube $[0,1]^s$. It first introduces the by-now standard setting of weighted Hilbert spaces of functions with square-integrable mixed first derivatives, and then indicates alternative settings, such as non-Hilbert spaces, that can sometimes be more suitable. Original contributions include the extension of the fast CBC ("component-by-component") construction of lattice rules that achieve the optimal convergence order (i.e., a rate of almost $1/N$, where N is the number of points, independently of dimension) to so-called POD ("product-and-order-dependent") weights, as seen in some recent applications. Although the paper has a strong focus on lattice rules, the function space settings are applicable to all QMC methods. Furthermore, the error analysis and construction of lattice rules can be adapted to polynomial lattice rules from the family of digital nets.

Contents

1 Introduction and some QMC basics

Quasi-Monte Carlo (QMC) methods are deterministic methods for high-dimensional integration that aim to outperform the classical Monte Carlo method. In the last 15 years great progress has been made, often in the setting of "worst-case" errors in a "weighted" Hilbert space, as introduced originally by Sloan and Woźniakowski in [53]. This we shall call the "standard setting", and a first aim of this paper is to explain that standard setting. But much of the paper will be concerned with extensions that go beyond the standard setting. These extensions include non-Hilbert space settings, infinite dimensional problems, and non-standard choices of "weights".

The paper is in part motivated by a recent application [31] by the present authors of QMC methods to the computation of expected values of functionals of the solutions of second-order partial differential equations with random coefficients. While we will not review the paper [31] here, that work encouraged us to look beyond the standard setting. For instance, the dimensionality in that problem is not just high, but truly infinite. And the weights that we are led to use are certainly non-standard (see §1.4). And although that paper in its final form is concerned with the particular kind of QMC method known as *lattice rules*, and stayed within a Hilbert space setting, in the course of the research we considered many other possibilities, and still believe that other QMC methods and non-Hilbert space settings offer exciting possibilities for this and other applications.

For the majority of this article we will focus on the integration problem over the s-dimensional unit cube

$$I_s(F) = \int_{[0,1]^s} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,, \tag{1}$$

with the dimensionality s being large but finite. Here F is a function which is Lebesgue integrable over $[0,1]^s$ with some extra smoothness so that in particular evaluations of F at points in $[0,1]^s$ are well-defined. An N-point QMC approximation to the integral (1) is an equal-weight quadrature rule of the form

$$Q_{s,N}(F) = \frac{1}{N}\sum_{i=1}^{N} F(\boldsymbol{y}^{(i)})\,, \tag{2}$$

with a well chosen set of points $\mathcal{P} = \{\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(N)}\} \subset [0,1]^s$.

What is so good about QMC rules? Why not use, for example, a product of 1-dimensional Gauss rules? The short answer is that while product Gauss rules might work well, and indeed might be the recommended option when s is small and F is sufficiently smooth (see, for example the book by Stroud [58]), every product rule is infeasible when s is large. Suppose for example that $s = 100$. Then even a product of 2-point rules will require 2^{100} points, a number of points that is certain to be beyond our reach for many lifetimes. This is a manifestation of the famous *curse of dimensionality* [2].

But even if product rules are excluded, why do we restrict ourselves to equal weights? The QMC rules integrate constants exactly, but in general fail to integrate exactly all polynomials of higher degree. Perhaps if we allowed the weights to be unequal we could integrate exactly at least some higher degree polynomials? Once again the curse of dimensionality is against us: for example if we want to integrate exactly all multilinear polynomials (that is, all functions that are linear with respect to each variable y_j) then we must

satisfy 2^s independent conditions. But perhaps the real reason for using equal weights is that this is the simplest choice to analyse.

Error bounds for QMC methods generally take the form of an inequality

$$|I_s(F) - Q_{s,N}(F)| \le D(\mathcal{P})\, V(F)\,, \tag{3}$$

in which the first factor, a *discrepancy*, is independent of F, and is a measure of the quality of the point set $\mathcal{P}$, while the second factor is independent of the point set, and is a measure of the difficulty of the integrand F. The prototype of such inequalities is the *Koksma-Hlawka inequality*, which we shall review briefly in §1.3. An inequality of this form has the nice feature that, for a given function F, the error bound will be reduced to the extent that we can reduce the discrepancy of the point set $\mathcal{P}$. (Note, however, that the error itself might *not* be reduced – the guarantee is only about the error bound.)

Much of the literature of QMC methods talks about *worst-case error*, not discrepancy. It may help to avoid later pain to realize that they usually refer to the same thing. To define worst-case error, suppose that the integrand F is constrained to lie in some Banach space $\mathcal{W}$ with norm $\|F\|_{\mathcal{W}}$. (The choice of function space is limited by the natural requirement that pointwise function values make sense. We will see many examples later. For now think of $s = 1$, and take either $\mathcal{W} = C[0,1]$ or $\mathcal{W} = H^1[0,1]$, the space of square-integrable functions on $[0,1]$, with some appropriate norm in $H^1[0,1]$, see §1.1 below for an example.) Then the worst-case error is defined by

$$e^{\mathrm{wor}}(\mathcal{P};\mathcal{W}) := \sup\{|I_s(F) - Q_{s,N}(F)| : \|F\|_{\mathcal{W}} \le 1\}\,. \tag{4}$$

It follows, since the error depends linearly on $\|F\|_{\mathcal{W}}$, that for all $F \in \mathcal{W}$ we have

$$|I_s(F) - Q_{s,N}(F)| \le e^{\mathrm{wor}}(\mathcal{P},\mathcal{W})\, \|F\|_{\mathcal{W}}\,, \tag{5}$$

which is of the same form as (3), with the discrepancy replaced by the worst-case error, and $V(F)$ replaced by the norm $\|F\|_{\mathcal{W}}$. Often $V(F)$ is a seminorm rather than a norm, but the distinction is often unimportant. (We could equally well use a seminorm in the definition of the worst-case error, but it would be non-standard to do so.) If $D(\mathcal{P})$ is the smallest possible constant in (3) and $V(F)$ is a norm or seminorm, then $D(\mathcal{P})$ is indeed a worst-case error.

1.1 The standard setting for QMC

In the *standard setting*, introduced in [53], the quantity $V(F)$ is a norm in a Hilbert space $\mathcal{H}_{s,\boldsymbol{\gamma}}$ of functions F that enjoy some smoothness and all of

whose mixed first derivatives are square-integrable over $[0,1]^s$; and these norms also incorporate *weights*, which are positive numbers $\gamma_1, \gamma_2, \ldots, \gamma_s$ designed to quantify the different degrees of difficulty associated with the different components of $\boldsymbol{y}$ in (1). We will always assume that

$$\gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_s > 0\,, \tag{6}$$

corresponding to the idea that the first component of $\boldsymbol{y}$ is the hardest one for this integrand, the second component the next hardest, and so on. For $s = 1$, the (real) space $\mathcal{H}_{1,\gamma_1}$ consists of absolutely continuous functions whose first derivatives are integrable. The inner product in $\mathcal{H}_{1,\gamma_1}$ is

$$\langle F, G\rangle_{1,\gamma_1} := F(1)\,G(1) + \frac{1}{\gamma_1}\int_0^1 F'(y)\,G'(y)\,\mathrm{d}y\,,\ F, G \in \mathcal{H}_{1,\gamma_1}\,,$$

thus the corresponding norm squared is

$$\|F\|^2_{1,\gamma_1} = |F(1)|^2 + \frac{1}{\gamma_1}\int_0^1 |F'(y)|^2\,\mathrm{d}y\,, \quad F \in \mathcal{H}_{1,\gamma_1}. \tag{7}$$

For $s = 2$, $\mathcal{H}_{2,\boldsymbol{\gamma}}$ is the tensor product of $\mathcal{H}_{1,\gamma_1}$ and $\mathcal{H}_{1,\gamma_2}$, and the norm squared in $\mathcal{H}_{2,\boldsymbol{\gamma}}$ (we leave the inner product to be inferred from the norm) is defined by

$$\begin{aligned}\|F\|^2_{2,\boldsymbol{\gamma}} := {}& |F(1,1)|^2 \\ &+ \frac{1}{\gamma_1}\int_0^1 \left|\frac{\partial F}{\partial y_1}(y_1,1)\right|^2 \mathrm{d}y_1 + \frac{1}{\gamma_2}\int_0^1 \left|\frac{\partial F}{\partial y_2}(1,y_2)\right|^2 \mathrm{d}y_2 \\ &+ \frac{1}{\gamma_1\gamma_2}\int_{[0,1]^2} \left|\frac{\partial^2 F(y_1,y_2)}{\partial y_1 \partial y_2}\right|^2 \mathrm{d}y_1\mathrm{d}y_2\,.\end{aligned}$$

Note that a small value of γ_2 forces the partial derivative $\frac{\partial F}{\partial y_2}$ to be small if F is to stay within the unit ball in $\mathcal{H}_{2,\boldsymbol{\gamma}}$.

The point of this definition of $\|F\|_{2,\boldsymbol{\gamma}}$ is that it matches the tensor product structure: for the special case $F(y_1, y_2) = G(y_1)H(y_2)$ it is easily seen that $\|F\|_{2,\boldsymbol{\gamma}} = \|G\|_{1,\gamma_1}\|H\|_{1,\gamma_2}$.

For general s, $\mathcal{H}_{s,\boldsymbol{\gamma}}$ is the tensor product of $\mathcal{H}_{1,\gamma_1} \otimes \mathcal{H}_{1,\gamma_2} \otimes \cdots \otimes \mathcal{H}_{1,\gamma_s}$, and we can write the norm squared in the more compact form

$$\|F\|^2_{s,\boldsymbol{\gamma}} := \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \left|\frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}\,, \tag{8}$$

where $\{1:s\} := \{1, \ldots, s\}$, so that the sum is over all subsets $\mathfrak{u}$ of $\{1, \ldots, s\}$, with $\boldsymbol{y}_{\mathfrak{u}}$ denoting the components y_j of $\boldsymbol{y}$ with $j \in \mathfrak{u}$, and with $(\boldsymbol{y}_{\mathfrak{u}}, 1)$ denoting

the vector of length s whose jth component is y_j if $j \in \mathfrak{u}$ and is 1 if $j \notin \mathfrak{u}$, and where $\gamma_{\mathfrak{u}}$ denotes the product

$$\gamma_{\mathfrak{u}} := \prod_{j \in \mathfrak{u}} \gamma_j \,. \tag{9}$$

Weights of this kind are nowadays referred to as "product" weights. In [53] it was assumed that $\gamma_1 = 1$, but this assumption is now considered to be unnecessary and too restrictive.

A short history of the standard setting is that the 1998 paper [53] proved non-constructively that for each $N \geq 1$ there exist QMC points $\{\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(N)}\} \subset [0,1]^s$ for which the worst-case error is bounded by $c/\sqrt{N}$, with c independent of s, if and only if

$$\sum_{j=1}^{\infty} \gamma_j < \infty \,. \tag{10}$$

Then in 2000 Hickernell and Woźniakowski in [21] proved (again non-constructively) that the bound can be improved to $c_\delta/N^{1-\delta}$ for arbitrary $\delta > 0$ under a stronger condition on the weights, most simply that

$$\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty. \tag{11}$$

The paper [54] then showed that there exists a QMC rule for which the worst-case error has a bound of the form $c_\delta/N^{1-\delta}$ even if the choice of QMC rule is restricted to the relatively small class of *shifted lattice rules*, see §1.2. The proof, like that in [53], uses an averaging argument (that there is at least one choice as good as the average) and is non-constructive. In 2002 Sloan, Kuo and Joe in [49] devised a *component-by-component* (or CBC) construction of a shifted lattice rule that for N prime achieves the $c/\sqrt{N}$ bound for the worst-case error in the standard setting, thereby achieving for prime N a constructive proof of the result in [53]. In [50] the same authors proposed a randomised version of the CBC construction, which was shown subsequently by Kuo [30] and Dick [5] to achieve the $c_\delta/N^{1-\delta}$ bound under the condition (11). Fast implementations of CBC constructions were introduced by Nuyens and Cools in [42] and [43], while modified algorithms for obtaining lattice rules that are extensible in N were given in [4] and [7]. These made feasible the construction of explicit lattice rules that match the rates of convergence of the worst-case error in the existence results for all values of s and N that are likely to be of interest.

1.2 Lattice methods

Much of this review will focus on an important family of QMC rules called *shifted lattice rules*. They take the form

$$Q_{s,N}(F) = \frac{1}{N}\sum_{i=1}^{N} F\left(\left\{\frac{i\boldsymbol{z}}{N} + \boldsymbol{\Delta}\right\}\right), \tag{12}$$

where $\boldsymbol{z} \in \mathbb{N}^s$ is known as the *generating vector*, $\boldsymbol{\Delta} \in [0,1]^s$ is the *shift*, and the braces around $\{\boldsymbol{w}\}$ mean to take the fractional part of each component of the vector $\boldsymbol{w}$. Shifted lattice rules therefore require the specification of two vector quantities: an integer vector $\boldsymbol{z} \in \mathbb{N}^s$, and a real number vector $\boldsymbol{\Delta} \in [0,1]^s$.

Lattice rules without shift, i.e., $\boldsymbol{\Delta} = \boldsymbol{0}$, were originally introduced in a periodic function space setting, see for example [48], but by now are seen to have an important role even for non-periodic spaces. In the last formula $\boldsymbol{\Delta}$ is deterministic. In contrast, a *randomly shifted* lattice rule takes the same form (12) in which as before $\boldsymbol{z} \in \mathbb{N}^s$ is a prescribed generating vector, but now each component of $\boldsymbol{\Delta} \in [0,1]^s$ is a random variable uniformly and independently distributed in $[0,1]$. Randomly shifted lattice rules have come to play an important role, as we foreshadowed in §1.1.

From a practical point of view there are multiple advantages in using a randomized QMC rule: while enjoying nearly the optimal rate of convergence, a randomly shifted lattice rule is unbiased and provides a simple and practical error estimation, just like the Monte Carlo method. (See [9, Section 5] for a brief explanation of how this error estimation is done in practice.)

The *component-by-component* (or CBC) algorithm was invented for periodic spaces by Korobov [29] many years ago, and rediscovered by Sloan and Reztsov in [51]. The subsequent developments in the non-periodic setting have already been foreshadowed in §1.1.

In the CBC algorithm the integers $z_1, \ldots, z_s$ are chosen one at a time, in the natural order. Suppose that $z_1, \ldots, z_{s-1}$ are already determined. Then z_s is determined by minimising a certain quantity (the *shift-averaged worst-case error*) over the (at most $N-1$) possible values of $1 \le z_s \le N-1$ that are coprime with N. For further details about the CBC algorithm, see §4.

1.3 The classical setting and what goes wrong

Here we briefly review the "classical" theory for obtaining bounds of the QMC error for non-periodic functions, and explain the problem with its applicability in high dimensions. (For functions that are 1-periodic with respect

to each of the s variables there is a theory based on Fourier analysis – see [36] and [48]. We shall not discuss the periodic case in this review.)

As foreshadowed in §1, the Koksma-Hlawka inequality plays an important role classically. This inequality takes the form

$$|I_s(F) - Q_{s,N}(F)| \le D^*(\mathcal{P})\, V_{\rm HK}(F)\,. \tag{13}$$

Here $V_{\rm HK}(F)$ is the *variation of F in the sense of Hardy and Krause*, see e.g. [36], and $D^*(\mathcal{P})$ is the (classical) *star discrepancy* of the QMC set $\mathcal{P} = \{\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(N)}\}$, defined by

$$D^*(\mathcal{P}) := \sup_{\boldsymbol{y}\in[0,1]^s} |{\rm discr}_{\mathcal{P}}(\boldsymbol{y})|\,,$$

where ${\rm discr}_{\mathcal{P}}(\cdot)$ is the *local discrepancy function*

$${\rm discr}_{\mathcal{P}}(\boldsymbol{y}) := y_1 y_2 \cdots y_s - \frac{\big|\{i : \boldsymbol{y}^{(i)} \in [0,\boldsymbol{y})\}\big|}{N}\,,\ \boldsymbol{y} \in [0,1]^s\,, \tag{14}$$

with $[0,\boldsymbol{y}) := [0,y_1)\times[0,y_2)\times\cdots\times[0,y_s)$. We shall discuss and prove more general versions of the Koksma-Hlawka inequality in §3.1.

The local discrepancy function is the difference between the volume of the rectangular region $[0,\boldsymbol{y})$ and the fraction of the QMC points that lie in the region. Intuitively, a small value of star discrepancy means that the points are closer to being uniformly distributed.

By definition, an infinite sequence of points $\boldsymbol{y}^{(1)}, \boldsymbol{y}^{(2)}, \ldots$ in $[0,1]^s$ is a *low-discrepancy sequence* if for arbitrary $N \ge 1$ the star discrepancy of its first N members satisfies

$$D^*(\mathcal{P}) \le C\,\frac{(\ln N)^s}{N}\,, \tag{15}$$

for some constant $C > 0$ which is independent of N but may depend on s. Examples of low-discrepancy sequences include *Halton sequences* [11], *Sobol′ sequences* [55], *Faure sequences* [8], *Niederreiter sequences* [35, 36], and *Niederreiter-Xing sequences* [37].

Although a bound of the form (15) indicates an ultimate order of convergence theoretically higher than the classical Monte Carlo rate of $1/\sqrt{N}$, that bound is unsatisfactory when the dimensionality is high because, for fixed s, $(\ln N)^s/N$ keeps growing with increasing N until N is exponentially large in s.

In contrast to that somewhat negative observation is a remarkable result proved in [12], that there exists a sequence of QMC point sets for which the star discrepancy is of order $\sqrt{s/N}$ (with an unknown constant), or alternatively, $\sqrt{s\ln s\,\ln N/N}$ (with an explicit constant). However, no-one yet knows how to construct QMC points that satisfy a bound of this kind.

1.4 Why go beyond the standard setting?

Within the standard setting we now know (see §1.1) that, with the help of suitable weights, we can obtain close to order $1/N$ for the worst-case error, with an implied constant independent of the dimension s, so allowing QMC methods to be applicable to really high-dimensional problems. Why might one want to go beyond the standard setting? One argument concerns the choice of weights. While the theoretical results concerning weights in §1.1 might be considered interesting, there have been few if any convincing prescriptions of the weights to use in any particular application: in most applications the choice of weights has been *ad hoc*. In the paper [31], in contrast, the choice of weights is an essential ingredient in the analysis. Interestingly, the weights found there turn out to be *not* of the product form (9), but are rather of "product-and-order-dependent" or "POD" form, in general defined by

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j\in\mathfrak{u}} \gamma_j \,, \tag{16}$$

where $|\mathfrak{u}|$ denotes the cardinality, or the *order*, of $\mathfrak{u}$. The multiplier $\Gamma_{|\mathfrak{u}|}$ in front of the product is a positive number that depends only on the order $|\mathfrak{u}|$ of the subset $\mathfrak{u}$, hence is said to be *order-dependent*. In the particular application in [31] the multiplier $\Gamma_{|\mathfrak{u}|}$ is found to be $\Gamma_{|\mathfrak{u}|} = (|\mathfrak{u}|!)^\nu$ for some positive number ν that is independent of $\mathfrak{u}$. Thus for the problem considered in [31] confining ourselves to product weights, see (9), is no longer reasonable. In the following subsection we shall see another example, this time a simple one, in which it is again true that the best weights are POD weights. Fortunately, a general notion of weights (in which at the extreme all of the 2^s weights $\gamma_{\mathfrak{u}}$ in (8) are chosen independently) has already been proposed in [52]. An efficient CBC construction is not available for all general weights, but an efficient CBC construction can be devised for the particular case of POD weights, as we shall show, as a new result, in §5 ahead.

Sometimes the Hilbert space aspect of the standard setting is a major restriction. This is often the case for problems whose natural setting is $\mathbb{R}^s$. For simplicity, we think for a moment of functions in only one dimension, that is $s = 1$. Then an integral of the form

$$\mathcal{I}_1(f) := \int_{-\infty}^{\infty} f(x)\,\rho(x)\,\mathrm{d}x \,,$$

where ρ is a given probability density function on $\mathbb{R}$, can be reformulated as a problem on the unit cube by the transformation

$$y = \Phi(x) := \int_{-\infty}^{x} \rho(t)\,\mathrm{d}t \,,$$

under which the integral $\mathcal{I}_1(f)$ becomes

$$\mathcal{I}_1(f) = \int_0^1 F(y)\,\mathrm{d}y = I_1(F)\,, \quad \text{with} \quad F(y) = f(\Phi^{-1}(y))\,.$$

But the resulting integrand lies in our space $\mathcal{H}_{1,\gamma_1}$, with its norm defined by (7), if and only if $F' \in L^2[0,1]$, where by the chain rule

$$F'(y) = \frac{f'(x)}{\Phi'(x)} = \frac{f'(\Phi^{-1}(y))}{\rho(\Phi^{-1}(y))}\,.$$

The problem comes from the requirement to square the denominator $\rho(x)$: it is often the case that the resulting integral

$$\int_0^1 |F'(y)|^2\,\mathrm{d}y = \int_0^1 \left|\frac{f'(\Phi^{-1}(y))}{\rho(\Phi^{-1}(y))}\right|^2 \mathrm{d}y = \int_{-\infty}^{\infty} \frac{|f'(x)|^2}{\rho(x)}\,\mathrm{d}x$$

diverges. In contrast, if the requirement were merely that $F' \in L^1[0,1]$, then the demand would be merely

$$\int_0^1 |F'(y)|\,\mathrm{d}y = \int_{-\infty}^{\infty} |f'(x)|\,\mathrm{d}x < \infty\,,$$

which is much more commonly satisfied.

We shall discuss more general Banach space settings in §3 (which may be viewed as a "second course" on QMC).

There is another important family of QMC methods called *digital nets*, see [36]. We shall not discuss results relating to digital nets in this review. For recent developments of digital nets, including analysis in weighted spaces and constructions that achieve higher order convergence (i.e., a convergence rate of order $N^{-\alpha}$ for $\alpha > 1$), we refer the reader to the recent book by Dick and Pillichshammer [6].

1.5 A new kind of example

Suppose that

$$a(\boldsymbol{y}) = a(y_1, \ldots, y_s) := 1 + \sum_{j=1}^{s} \frac{y_j^\alpha}{j^2}\,, \tag{17}$$

is a physical quantity that depends on s independent random variables $y_1, \ldots, y_s$, each uniformly distributed over $[0,1]$, and that $0 < \alpha \le 1$. We note that

$$1 \le a(\boldsymbol{y}) \le 1 + \sum_{j=1}^{\infty} \frac{1}{j^2} = 1 + \frac{\pi^2}{6} \quad \forall \boldsymbol{y} \in [0,1]^s, \quad \forall s \ge 1\,.$$

Our problem is to find the expected value of the reciprocal of a,

$$F(\boldsymbol{y}) := \frac{1}{a(\boldsymbol{y})}\,. \tag{18}$$

Since the y_j are i.i.d. uniform over $[0,1]$, this expectation is given by

$$I_s(F) = \int_{[0,1]^s} \frac{1}{a(\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y} = \int_0^1 \cdots \int_0^1 \frac{1}{a(y_1,\ldots,y_s)}\,\mathrm{d}y_1 \ldots \mathrm{d}y_s\,.$$

It is easily verified that $I_s(F)$ is well-defined for $\alpha > 0$.

The integrand $F(\boldsymbol{y})$ is a simplified model of an elliptic partial differential equation with a random coefficient, as studied in [31]. Though the latter problem is beyond the scope of this paper, there as here the variables $y_1, y_2, \ldots$ are parameters in a "probability space". The big difference in that problem is the presence of another variable $\boldsymbol{x} \in \mathbb{R}^2$ or $\mathbb{R}^3$ corresponding to position in physical space; and that one has to solve an elliptic PDE with respect to the physical variable $\boldsymbol{x}$.

If we write the definition (18) instead as an algebraic equation,

$$a(\boldsymbol{y})F(\boldsymbol{y}) = 1,$$

then the present example has the flavour of the elliptic PDE considered in [31], while avoiding all PDE complications.

Suppose that we want to approximate $I_s(F)$ by a randomly shifted lattice rule, see (12). Then obviously we need to know a good choice for the integer vector $\boldsymbol{z}$. In turn, if we want to generate a good choice of $\boldsymbol{z}$ by the CBC algorithm (see §1.2 and §4) then we need to know a good choice of the weights $\gamma_{\mathfrak{u}}$ to steer the CBC algorithm.

The first step towards a rational choice of weights is to determine (or obtain a bound on) the norm $\|F\|_{s,\boldsymbol{\gamma}}$. To this end, by direct differentiation of F we easily find, with $d_j := \alpha/j^2$,

$$\frac{\partial F}{\partial y_j} = -\frac{d_j y_j^{\alpha-1}}{[a(\boldsymbol{y})]^2}, \quad 1 \le j \le s\,,$$

$$\frac{\partial^2 F}{\partial y_j y_k} = \frac{2\,d_j d_k (y_j y_k)^{\alpha-1}}{[a(\boldsymbol{y})]^3}, \quad 1 \le j,k \le s,\ j \ne k\,,$$

and for the mixed first partial derivative with respect to the variables with labels in $\mathfrak{u}$,

$$\frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}} = \frac{|\mathfrak{u}|!\,\prod_{j\in\mathfrak{u}}(-d_j y_j^{\alpha-1})}{[a(\boldsymbol{y})]^{|\mathfrak{u}|+1}}\,.$$

Hence, on using $a(\boldsymbol{y}) \ge 1$ we find, for $\alpha > 1/2$,

$$\int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \le \frac{(|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} d_j^2}{(2\alpha-1)^{|\mathfrak{u}|}},$$

and on defining $b_j := d_j/(\sqrt{2\alpha-1}) = \alpha/(j^2\sqrt{2\alpha-1})$, we obtain a bound on the norm (8),

$$\|F\|_{s,\boldsymbol{\gamma}}^2 \le \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}}. \tag{19}$$

We observe that, as $\alpha \to 1/2$, the bound approaches infinity, even though the expectation of $1/a(\boldsymbol{y})$ is well defined for all $0 < \alpha \le 1$. We thus see that non-Hilbert space norms might be advantageous in order to cover as wide a class of integrands as possible. This is one motivation for considering the Banach space setting in §3 ahead.

Given the bound (19) on the norm, how can we decide on the best choice of weights $\gamma_{\mathfrak{u}}$, and go on to obtain an error bound for $|I_s(F) - Q_{s,N}(F)|$? The principle used in [31] is that *we should choose weights that as far as possible minimize the error bound* (5). Bearing in mind the upper bound (19), that means we should choose weights that minimize the right-hand side of

$$|I_s(F) - Q_{s,N}(F)| \le e^{\mathrm{wor}}(\mathcal{P}; \mathcal{H}_{s,\boldsymbol{\gamma}}) \left(\sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}} \right)^{1/2}. \tag{20}$$

We shall show later in §4, see Theorem 5, that if $Q_{s,N}$ is a randomly shifted lattice rule constructed by the CBC algorithm, and if we interpret the error in (20) as the root-mean-square error averaged over shifts, then the right-hand side of (20) can be further bounded (for the simplest case of prime N) by

$$\left(\frac{2}{N} \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} (\rho(\lambda))^{|\mathfrak{u}|} \right)^{1/(2\lambda)} \left(\sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}} \right)^{1/2}, \tag{21}$$

where

$$\rho(\lambda) := \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} + \left(\frac{1}{3}\right)^{\lambda}.$$

Here $\zeta(x) := \sum_{k=1}^{\infty} 1/k^x$ for $x > 1$ is the Riemann zeta function, and λ is any number satisfying $1/2 < \lambda \le 1$. Obviously we get the best rate of convergence, a rate close to $1/N$, by taking λ close to $1/2$, but λ must remain strictly greater than $1/2$ because $\zeta(x) \to \infty$ as $x \to 1$.

In [31, Theorem 6.3] it is shown (and the reader can easily verify by simple calculus) that (21) is minimized, and bounded independently of s, by choosing the weights to be

$$\gamma_{\mathfrak{u}} = \left(|\mathfrak{u}|! \prod_{j \in \mathfrak{u}} \frac{b_j}{\sqrt{\rho(\lambda)}} \right)^{\frac{2}{1+\lambda}} .$$

Thus the best choice of weights, in the sense of minimising the error bound, is a POD ("product-and-order-dependent") weight, and this choice gives a rate of convergence that is independent of s, and arbitrarily close to $1/N$ when λ is close to $1/2$.

2 QMC in a Hilbert space setting

In the standard setting, as described in §1.1, the function space $\mathcal{W}_{s,\boldsymbol{\gamma}}$ is a special kind of Hilbert space called a *reproducing kernel Hilbert space*, or RKHS, see [1]. Such Hilbert spaces are often useful in numerical analysis, since a Hilbert space is an RKHS if and only if point evaluation is a bounded linear functional. It turns out that the error analysis for numerical integration in general, and QMC integration in particular, is especially simple in an RKHS setting. In this section we describe that error analysis, then apply it to the standard setting.

2.1 Reproducing kernel Hilbert spaces

A Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot, \rangle_{\mathcal{H}}$ is an RKHS, see [1], if and only if there is a unique function $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$, referred to as the *reproducing kernel*, with the following properties:

$$K(\boldsymbol{y}, \cdot) \in \mathcal{H} \quad \text{for all } \boldsymbol{y} \in [0,1]^s ,$$

$$K(\boldsymbol{y}, \boldsymbol{y}') = K(\boldsymbol{y}', \boldsymbol{y}) \quad \text{for all } \boldsymbol{y}, \boldsymbol{y}' \in [0,1]^s ,$$

$$F(\boldsymbol{y}) = \langle F, K(\boldsymbol{y}, \cdot) \rangle_{\mathcal{H}} \quad \text{for all } \boldsymbol{y} \in [0,1]^s \text{ and } F \in \mathcal{H} . \tag{22}$$

The last property is known as the reproducing property. The existence of the reproducing kernel is a consequence of the boundedness of point evaluation, as follows from the Riesz representation theorem, see [1].

The RKHS approach provides a very powerful tool for obtaining QMC error bounds, provided the kernel is known, and available in closed form. (This is certainly the case for the standard setting – see (25) below.) This

is because, as we shall now show, there is a simple but completely general expression for the worst-case error in terms of the reproducing kernel. Thus the worst-case error in an RKHS has an explicit formula.

2.2 Worst-case error in an RKHS

Suppose $\mathcal{H}$ is an RKHS with reproducing kernel $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$. Using (2) and the reproducing property (22) we can write

$$Q_{s,N}(F) = \frac{1}{N}\sum_{i=1}^{N}\langle F, K(\boldsymbol{y}^{(i)},\cdot)\rangle_{\mathcal{H}} = \left\langle F, \frac{1}{N}\sum_{i=1}^{N} K(\boldsymbol{y}^{(i)},\cdot)\right\rangle_{\mathcal{H}}.$$

In a similar way, any bounded linear functional T on $\mathcal{H}$ can be represented as $T(F) = \langle F, \tilde{T}\rangle_{\mathcal{H}}$, with $\tilde{T}(\boldsymbol{y}) = T(K(\boldsymbol{y},\cdot))$ for all $\boldsymbol{y} \in [0,1]^s$. Assuming that I_s is a bounded linear functional on $\mathcal{H}$ (which will always be the case for the spaces of interest to us), we can thus write

$$I_s(F) = \left\langle F, \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,\mathrm{d}\boldsymbol{y}\right\rangle_{\mathcal{H}},$$

and hence by subtraction,

$$I_s(F) - Q_{s,N}(F) = \langle F, \xi_{s,N}\rangle_H\,, \tag{23}$$

where $\xi_{s,N}$ is the *representer* of the error,

$$\begin{aligned}\xi_{s,N}(\boldsymbol{y}') :=& I_s(K(\cdot,\boldsymbol{y}')) - Q_{s,N}(K(\cdot,\boldsymbol{y}'))\\ =& \int_{[0,1]^s} K(\boldsymbol{y},\boldsymbol{y}')\,\mathrm{d}\boldsymbol{y} - \frac{1}{N}\sum_{i=1}^{N} K(\boldsymbol{y}^{(i)},\boldsymbol{y}')\,.\end{aligned}$$

By the Cauchy-Schwarz inequality, we obtain from (23) the error bound

$$|I_s(F) - Q_{s,N}(F)| = |\langle F, \xi_{s,N}\rangle_{\mathcal{H}}| \le \|F\|_{\mathcal{H}}\|\xi_{s,N}\|_{\mathcal{H}}\,.$$

Equality holds when F is a multiple of $\xi_{s,N}$, thus by the definition of worst-case error (4) we see that

$$e^{\mathrm{wor}}(\mathcal{P};\mathcal{H}) = \|\xi_{s,N}\|_{\mathcal{H}}.$$

This leads us to the following explicit formula for the worst-case error.

Lemma 1 *If $\mathcal{H}$ is an RKHS with reproducing kernel K, and if I_s is a bounded linear functional on $\mathcal{H}$, then*

$$[e^{\rm wor}(\mathcal{P};\mathcal{H})]^2 = \int_{[0,1]^s} \left(\int_{[0,1]^s} K(\boldsymbol{y},\boldsymbol{y}')\,{\rm d}\boldsymbol{y} \right) {\rm d}\boldsymbol{y}' - \frac{2}{N}\sum_{i=1}^N \int_{[0,1]^s} K(\boldsymbol{y}^{(i)},\boldsymbol{y})\,{\rm d}\boldsymbol{y} + \frac{1}{N^2}\sum_{i=1}^N\sum_{i'=1}^N K(\boldsymbol{y}^{(i)},\boldsymbol{y}^{(i')})\,.$$

Proof: Using the reproducing property of $K(\cdot,\cdot)$ and the linearity of $I_s(\cdot)$ and $Q_{s,N}(\cdot)$, we obtain

$$[e^{\rm wor}(\mathcal{P};\mathcal{H})]^2 = \left\| \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y} - \frac{1}{N}\sum_{i=1}^N K(\boldsymbol{y}^{(i)},\cdot) \right\|_{\mathcal{H}}^2$$

$$= \left\langle \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y} - \frac{1}{N}\sum_{i=1}^N K(\boldsymbol{y}^{(i)},\cdot)\,,\ \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y} - \frac{1}{N}\sum_{i=1}^N K(\boldsymbol{y}^{(i)},\cdot) \right\rangle_{\mathcal{H}}$$

$$= \left\langle \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y}, \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y} \right\rangle_{\mathcal{H}} - \frac{2}{N}\sum_{i=1}^N \left\langle \int_{[0,1]^s} K(\boldsymbol{y},\cdot)\,{\rm d}\boldsymbol{y}\,, K(\boldsymbol{y}^{(i)},\cdot) \right\rangle_{\mathcal{H}}$$
$$+ \frac{1}{N^2}\sum_{i=1}^N\sum_{i'=1}^N \left\langle K(\boldsymbol{y}^{(i)},\cdot), K(\boldsymbol{y}^{(i')},\cdot) \right\rangle_{\mathcal{H}}\,.$$

Using again the reproducing property (22), we obtain the desired formula. ♠

2.3 Error analysis in the standard setting

Recall that $\mathcal{H}_{s,\boldsymbol{\gamma}}$ denotes the Hilbert space in the standard setting of §1.1. Then the inner product corresponding to the norm (8) is

$$\langle F, G\rangle_{s,\boldsymbol{\gamma}} = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}},1)\,\frac{\partial^{|\mathfrak{u}|}G}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}},1)\,{\rm d}\boldsymbol{y}_{\mathfrak{u}}\,, \tag{24}$$

where $\gamma_{\mathfrak{u}}$ is again given by (9) and where the notation is as in (8).

It can be shown that the reproducing kernel for the space $\mathcal{H}_{s,\boldsymbol{\gamma}}$ is

$$K_{s,\boldsymbol{\gamma}}(\boldsymbol{y},\boldsymbol{y}') = \prod_{j=1}^s \left(1+\gamma_j\left[1-\max(y_j,y_j')\right]\right)\ ,\ \boldsymbol{y},\boldsymbol{y}'\in[0,1]^s\,. \tag{25}$$

(It is a useful exercise, based solely on integration by parts and the definition of the norm, to verify the reproducing property (22) for $s = 1$.) An explicit expression for the worst-case error of the space $\mathcal{H}_{s,\boldsymbol{\gamma}}$ is then given by Lemma 1 as

$$[e^{\mathrm{wor}}(\mathcal{P}; \mathcal{H}_{s,\boldsymbol{\gamma}})]^2 = \prod_{j=1}^{s} \left(1 + \frac{\gamma_j}{3}\right) - \frac{2}{N} \sum_{i=1}^{N} \prod_{j=1}^{s} \left(1 + \frac{\gamma_j}{2} \left(1 - [t_j^{(i)}]^2\right)\right) + \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} \prod_{j=1}^{s} \left(1 + \gamma_j \left(1 - \max(t_j^{(i)}, t_j^{(i')})\right)\right). \quad (26)$$

As we shall explain in §3, this quantity is also known by the name of "weighted L^2 discrepancy". (The unweighted version, i.e., $\gamma_j = 1$, is due to Warnock [60]; the weighted version was derived by Joe [25].)

This machinery provided the foundation for the series of developments foreshadowed in §1.1 and §1.2, from the non-constructive error bounds on general QMC methods, to the component-by-component (CBC) construction of randomly shifted lattice rules that achieve the $c_\delta/N^{1-\delta}$ bound with $\delta > 0$ arbitrary small (probabilistically, since the shift is random) under the condition (11). More details about the theory and construction of lattice rules will be given in §4 and §5.

3 Banach space settings with general weights

In this section we go beyond the standard setting in two ways. Firstly, we move away from Hilbert space settings to Banach space settings. Secondly, we consider general weights instead of product weights (9).

More precisely, we assume that the integrand F in (1) admits in particular *mixed first derivatives belonging to* L^q for some $q \in [1, \infty]$, and we define a norm by *combining the derivative terms in the* ℓ^r *sense* for $r \in [1, \infty]$. Denoting here the function space by $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$, we derive the *weighted Koksma-Hlawka inequality*

$$|I_s(F) - Q_{s,N}(F)| \le D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \, \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}}, \quad (27)$$

where q' and r' are the Hölder conjugates of q and r respectively, i.e., $1/q + 1/q' = 1$ and $1/r + 1/r' = 1$ for q and r strictly between 1 and ∞, and as usual 1 is the conjugate of ∞ and vice versa. For the precise definition of the norm $\|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}}$ and the discrepancy $D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P})$ see (30) and (31) below. For now it suffices to say that the $q = r = 2$ case corresponds to the standard

setting if we have product weights, while the $q = r = 1$ case corresponds to the classical setting if all weights are equal to 1.

We shall explain below that q and r play different roles in the QMC error bounds, and that *decoupling q and r allows for more flexibility in the QMC analysis.*

3.1 Deriving the weighted Koksma-Hlawka inequality

In this subsection we derive the generalized QMC error bound (27), a weighted version of the Koksma-Hlawka inequality (13). Like the Koksma-Hlawka inequality itself, this can be derived from the *Hlawka-Zaremba identity, [24] and* [61]. Assuming that the integrand F in (1) is sufficiently smooth, the identity states that

$$\begin{aligned} &I_s(F) - Q_{s,N}(F) \\ &= \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} (-1)^{|\mathfrak{u}|} \int_{[0,1]^{|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\, \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\, \mathrm{d}\boldsymbol{y}\,, \end{aligned} \tag{28}$$

where $\mathrm{discr}_{\mathcal{P}}(\cdot)$ is the local discrepancy function defined in (14) and the notation is the same as in (8).

The validity of the Hlawka-Zaremba identity is easily verified in the case $s = 1$: if we adopt the convention that

$$0 = y^{(0)} \leq y^{(1)} \leq \ldots \leq y^{(N)} \leq y^{(N+1)} = 1\,,$$

then the right hand side of the identity becomes

$$\begin{aligned} -\int_0^1 F'(y) \left(y - \frac{|i : y^{(i)} \in [0,y)|}{N} \right) \mathrm{d}y &= -\sum_{i=1}^{N+1} \int_{y^{(i-1)}}^{y^{(i)}} F'(y) \left(y - \frac{i-1}{N} \right) \mathrm{d}y \\ &= -\frac{1}{N} \sum_{i=1}^{N} F(y^{(i)}) + \int_0^1 F(y)\, \mathrm{d}y\,, \end{aligned}$$

where the last step comes from integration by parts and recombination of the terms. The general case follows in a similar way by recursively applying the preceding univariate integration by parts with respect to each coordinate y_j.

As in (24), we introduce weights $\gamma_{\mathfrak{u}}$ into the error bound, but now allowing a different positive weight $\gamma_{\mathfrak{u}}$ for each subset $\mathfrak{u} \subseteq \{1 : s\}$. For each term in the sum of (28), we multiply and divide by $\gamma_{\mathfrak{u}}^{1/2}$ to get

$$I_s(F) - Q_{s,N}(F)$$

$$= \sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} (-1)^{|\mathfrak{u}|} \int_{[0,1]^{|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\, \gamma_{\mathfrak{u}}^{-1/2} \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\, \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}\,.$$

Clearly nothing has been changed at this point. Next we use Hölder's inequality for integrals with the conjugate exponents q and q' to obtain

$$\begin{aligned} &|I_s(F) - Q_{s,N}(F)| \\ &\le \sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{-1/2} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^q} \left\| \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}\,, \end{aligned}$$

where the L^q norm of a function f is defined as usual by

$$\|f\|_{L^q} := \begin{cases} \left(\int_{[0,1]^s} |f(\boldsymbol{y})|^q \, \mathrm{d}\boldsymbol{y} \right)^{1/q} & \text{for} \quad q \in [1, \infty)\,, \\ \operatorname{ess\,sup}_{\boldsymbol{y} \in [0,1]^s} |f(\boldsymbol{y})| & \text{for} \quad q = \infty\,. \end{cases}$$

Then we use Hölder's inequality for sums with the conjugate pair r and r' to arrive at

$$\begin{aligned} |I_s(F) - Q_{s,N}(F)| \le &\left(\sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{-1/2} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^q}^r \right)^{1/r} \\ &\times \left(\sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r'} \right)^{1/r'}\,, \end{aligned} \tag{29}$$

with the usual modification for the case $r = \infty$ or $r' = \infty$.

The first factor in (29) prompts us to define our norm by, for $1 \le q \le \infty$,

$$\begin{aligned} &\|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}} \\ &:= \begin{cases} \left(\sum_{\mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{-1/2} \, \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^q}^r \right)^{1/r} & \text{for } 1 \le r < \infty\,, \\ \max_{\mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{-1/2} \, \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^q} & \text{for } r = \infty\,, \end{cases} \end{aligned} \tag{30}$$

and we denote by $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ the completion of the space $C^\infty([0,1]^s)$ under this norm. Note that we have added the $\mathfrak{u} = \emptyset$ term to the sum to make it a true norm. The expression without the $\mathfrak{u} = \emptyset$ term is a seminorm which is sometimes referred to as the *variation* of F. We define the second factor in (29) to be the *weighted discrepancy* of the QMC point set $\mathcal{P}$,

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P})$$

$$:= \begin{cases} \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r'} \right)^{1/r'} & \text{for } 1 \le r' < \infty \,, \\ \max_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}} & \text{for } r' = \infty \,. \end{cases} \tag{31}$$

With the definitions (30) and (31), we obtain the *weighted Koksma-Hlawka inequality* in (27).

The weighted Koksma-Hlawka inequality (29) was first derived by Sloan and Woźniakowski [53], but with q always equal to r. The unweighted version, i.e., all weights $\gamma_{\mathfrak{u}} = 1$, had appeared earlier in the QMC literature, but again seemingly always with $q = r$; it was derived by Zaremba [61] for $q = r = 2$ and by Sobol′ [56] for general $q = r$. The classical Koksma-Hlawka inequality can be recovered by taking the unweighted version with $q = r = 1$; it was proved by Koksma [28] for dimension $s = 1$ and generalized by Hlawka [23] for $s \ge 1$. Actually, the classical Koksma-Hlawka inequality in its original form has the *variation in the sense of Hardy and Krause* instead of the norm of F; this variation is precisely the norm without the $\mathfrak{u} = \emptyset$ term whenever all mixed first partial derivatives are continuous on $[0,1]^s$, see e.g., [36].

As an exercise, the reader might wish to check for which parameters q and r and which weights $\gamma_{\mathfrak{u}}$ the function $F(\boldsymbol{y})$ in §1.5 belongs to $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ and has its norm bounded independently of s.

3.2 Connection between discrepancy and worst-case error

It turns out that the weighted discrepancy $D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P})$ is precisely the worst-case error in the space $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$, indicating that the weighted Koksma-Hlawka inequality is tight.

Lemma 2 *Let $\mathcal{P}$ be a finite point set in $[0,1]^s$. Then*

$$e^{\mathrm{wor}}(\mathcal{P}; \mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}) = D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \,.$$

Proof: For a function F in the unit ball of $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$, the weighted Koksma-Hlawka inequality (27) yields

$$|I_s(F) - Q_{s,N}(F)| \le D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \,, \tag{32}$$

so to prove the lemma it would be sufficient to construct an integrand for which equality is attained in (32). This is possible for $q, r \ge 2$. For $q = 1$ or

$r = 1$ (i.e., $q' = \infty$ or $r' = \infty$), instead a "nearly worst-case" integrand F^ϵ is constructed for arbitrary $\epsilon > 0$, one for which

$$|I_s(F^\epsilon) - Q_{s,N}(F^\epsilon)| \geq D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) - \epsilon\,.$$

Under more general function space settings, this result is discussed in [13] for $q = r$ and in [17] for general q, r; a proof for $q = r = 1$ is given in [16] and a proof for $q, r \geq 2$ is given in [19]. ♠

3.3 Two special cases: $q = r = 2$ and $q = r = 1$

Most QMC analyses follow one of two approaches. The first approach uses the Hilbert space setting of $q = r = 2$, and studies the *weighted L^2 discrepancy* $D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})$. This has the nice explicit representation

$$[D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})]^2 = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \left[\frac{1}{3^{|\mathfrak{u}|}} - \frac{2}{N} \sum_{i=1}^{N} \prod_{j \in \mathfrak{u}} \frac{1 - [t_j^{(i)}]^2}{2} + \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} \prod_{j \in \mathfrak{u}} \Big(1 - \max(t_j^{(i)}, t_j^{(i')})\Big) \right], \tag{33}$$

which we met already for the product weight case as a worst-case error in (26). Two QMC constructions related to this formula are [49, 50].

The other important approach uses the non-Hilbert setting of $q = r = 1$ (and thus $q' = r' = \infty$) and so studies the *weighted star discrepancy*

$$\begin{aligned} D_{s,\boldsymbol{\gamma}}^{\infty,\infty}(\mathcal{P}) &= \max_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \sup_{\boldsymbol{y}_{\mathfrak{u}} \in [0,1]^{|\mathfrak{u}|}} \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \\ &= \sup_{\boldsymbol{y} \in [0,1]^s} \max_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \;=:\; D_{s,\boldsymbol{\gamma}}^{*}(\mathcal{P})\,, \end{aligned}$$

see e.g., [53, 59, 26, 22, 6]. (We remark that our scaling with weights $\gamma_{\mathfrak{u}}^{1/2}$ is consistent with [53, 59], but the scaling $\gamma_{\mathfrak{u}}$ was used in [26, 6].) Unlike the L^2 counterpart, there is no easy formula for computing the weighted star discrepancy for a given point set (except when the dimensionality s is as low as 2 or 3), and one must work with some form of upper bound. We will discuss recent constructive results from both approaches in §4.

3.4 The benefit of decoupling q and r

The idea of decoupling q and r originated from the works of Hickernell, Sloan and Wasilkowski [17, 19], who observed that since the L^q norm for a function

defined on the unit cube increases with increasing q, and the ℓ^r norm for a vector increases with decreasing r, we have the partial ordering

$$\|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{1,\infty}} \le \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q_1,r_1}} \le \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q_2,r_2}} \le \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{\infty,1}},$$

$$D_{s,\boldsymbol{\gamma}}^{\infty,1}(\mathcal{P}) \ge D_{s,\boldsymbol{\gamma}}^{q_1',r_1'}(\mathcal{P}) \ge D_{s,\boldsymbol{\gamma}}^{q_2',r_2'}(\mathcal{P}) \ge D_{s,\boldsymbol{\gamma}}^{1,\infty}(\mathcal{P}), \tag{34}$$

for all

$$\begin{cases} 1 \le q_1 \le q_2 \le \infty, \\ \infty \ge r_1 \ge r_2 \ge 1, \end{cases} \quad \begin{cases} \infty \ge q_1' \ge q_2' \ge 1, \\ 1 \le r_1' \le r_2' \le \infty. \end{cases}$$

This partial ordering implies the embedding

$$\mathcal{W}_{s,\boldsymbol{\gamma}}^{\infty,1} \subset \mathcal{W}_{s,\boldsymbol{\gamma}}^{q_2,r_2} \subset \mathcal{W}_{s,\boldsymbol{\gamma}}^{q_1,r_1} \subset \mathcal{W}_{s,\boldsymbol{\gamma}}^{1,\infty}$$

with continuous injections.

Thus in the weighted Koksma-Hlawka inequality (27) we are able to have a smaller norm paired with a larger discrepancy, or a larger norm paired with a smaller discrepancy. The trade-off between the norm and the discrepancy determines the final QMC error bound. It is therefore important to consider the norm and the discrepancy together, rather than focusing solely on the discrepancy (as is done in many QMC analyses).

We also see that decoupling q and r allows for more flexibility in the QMC analysis. Observe that the partial ordering (34) does not allow for a comparison between $D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})$ and $D_{s,\boldsymbol{\gamma}}^{\infty,\infty}(\mathcal{P})$ in general, thus the two special cases discussed in §3.3 have been treated separately in the past. However, if a given integrand can be bounded in a larger norm, say, $\mathcal{W}_{s,\boldsymbol{\gamma}}^{\infty,1}$, then the smaller discrepancy $D_{s,\boldsymbol{\gamma}}^{1,\infty}(\mathcal{P})$ can be used, and in this case all existing bounds on other larger discrepancies, including both $D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})$ and $D_{s,\boldsymbol{\gamma}}^{\infty,\infty}(\mathcal{P})$, can be applied.

3.5 The weighted space $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ and generalizations

It is easy to see that different values of the parameter r yield equivalent norms in the function space $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$, thus do not change the function space itself. However, as we shall see later in §3.9, *tractability* results can depend on the specific value of r.

In the norm (30), $\frac{\partial^{|\mathfrak{u}|}F}{\partial \boldsymbol{y}_{\mathfrak{u}}}$ is evaluated at $(\boldsymbol{y}_{\mathfrak{u}}, 1)$, meaning that the components of $\boldsymbol{y}$ with indices outside the set $\mathfrak{u}$ are replaced by 1. Instead we could use an arbitrary *anchor* $a \in [0,1]$ (the choice $a = 1/2$ is popular). There is also an *unanchored* variant which, instead of freezing a component at the anchor value, integrates a component out, see e.g., [52]. For simplicity we

shall consider in this paper only the anchored space, and only the anchor $a = 1$.

Since the integrals arising from practical problems are often formulated over $\mathbb{R}^s$ rather than the unit cube, the paper [32] considered a generalization of the function space for unbounded integrands in $\mathbb{R}^s$.

Earlier works by Hickernell [13, 14] considered unweighted spaces with general $q = r$, with a generalization of the function space that covers both the anchored and unanchored variants. Later works by Hickernell, Sloan and Wasilkowski [16, 17, 18, 19] considered weighted spaces with general anchor, general product domain, and general product measure; the papers [16, 18] focused on the case $q = r = 1$ while [17, 19] allowed for general q and r.

3.6 Anchored decomposition

Let $\mathcal{W}^{q,r}_{\mathfrak{u},\boldsymbol{\gamma}}$ denote the subspace of $\mathcal{W}^{q,r}_{s,\boldsymbol{\gamma}}$ containing functions $F(\boldsymbol{y})$ that depend only on the set of variables whose indices belong to a set $\mathfrak{u} \subseteq \{1:s\}$. Denote this set of variables by $\boldsymbol{y}_\mathfrak{u}$. Every function in $\mathcal{W}^{q,r}_{s,\boldsymbol{\gamma}}$ has a unique decomposition of the form

$$F(\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1:s\}} F_\mathfrak{u}(\boldsymbol{y}_\mathfrak{u})\,,$$

where $F_\mathfrak{u}$ belongs to the space $\mathcal{W}^{q,r}_{\mathfrak{u},\boldsymbol{\gamma}}$ and satisfies also the condition that for all $\mathfrak{u} \neq \emptyset$

$$F_\mathfrak{u}(\boldsymbol{y}_\mathfrak{u}) = 0 \quad \text{if} \quad y_j = 1 \quad \text{for any} \quad j \in \mathfrak{u}\,.$$

This is sometimes called the *anchored decomposition*. It was shown in [33] that an explicit formula for $F_\mathfrak{u}$ is given by

$$F_\mathfrak{u}(\boldsymbol{y}_\mathfrak{u}) = \sum_{\mathfrak{v}\subseteq\mathfrak{u}} (-1)^{|\mathfrak{u}|-|\mathfrak{v}|} F(\boldsymbol{y}_\mathfrak{v}, 1)\,.$$

Similar decompositions exist for a general anchor and other more general variants of the function space, see [33]. The best known of these decompositions is the ANOVA decomposition, see e.g., [3, 57].

From the anchored decomposition of F we have

$$\frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_\mathfrak{u}}(\boldsymbol{y}_\mathfrak{u}, 1) = \sum_{\mathfrak{u}'\subseteq\{1:s\}} \frac{\partial^{|\mathfrak{u}|} F_{\mathfrak{u}'}}{\partial \boldsymbol{y}_\mathfrak{u}}(\boldsymbol{y}_\mathfrak{u}, 1) = \frac{\partial^{|\mathfrak{u}|} F_\mathfrak{u}}{\partial \boldsymbol{y}_\mathfrak{u}}(\boldsymbol{y}_\mathfrak{u})\,.$$

The last equality holds because if there is an index $j \in \mathfrak{u}$ but $j \notin \mathfrak{u}'$, then $F_{\mathfrak{u}'}$ does not depend on y_j and its partial derivative with respect to y_j is 0; while if there is an index $j \in \mathfrak{u}'$ but $j \notin \mathfrak{u}$, then fixing y_j at 1 annihilates $F_{\mathfrak{u}'}$.

It then follows that the norm in $\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ can also be expressed, for $1 \le q \le \infty$ and $1 \le r < \infty$, in either of the forms

$$\|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}} = \left(\sum_{\mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{-1/2} \frac{\partial^{|\mathfrak{u}|} F_{\mathfrak{u}}}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}) \right\|_{L^q}^r \right)^{1/r} = \left(\sum_{\mathfrak{u} \subseteq \{1:s\}} \|F_{\mathfrak{u}}\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}}^r \right)^{1/r},$$

with the obvious modification for $r = \infty$. Hence we have a decomposition of the norm corresponding to the anchored decomposition. (Note that there needs to be a precise match between the chosen norm and the type of decomposition. For example, the unanchored variant of the norm should be combined with the ANOVA decomposition.)

It is generally too costly or even infeasible to compute the anchored decomposition of a given function F; however, the concept of an anchored decomposition is useful as a technical tool in QMC error analysis.

3.7 Extension of RKHS analysis to Banach space setting

As argued in [13], see also [14, Section 3.2], we can often extend by continuity the inner product $\langle \cdot, \cdot \rangle_{\mathcal{W}}$ defined on $\mathcal{W} \times \mathcal{W}$ to $\mathcal{H} \times \mathcal{J}$, where $\mathcal{H} \supset \mathcal{W}$, and $\mathcal{J} \subset \mathcal{W}$. This allows the RKHS machinery with a given reproducing kernel to be extended to Banach spaces. More specifically, we have from (23) and the definition of the inner product (24) that

$$\begin{aligned} I_s(F) - Q_{s,N}(F) &= \langle F, \xi_{s,N} \rangle_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{2,2}} \\ &= \sum_{\mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} F}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \, \frac{\partial^{|\mathfrak{u}|} \xi_{s,N}}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \, \mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \,. \end{aligned}$$

For any $\boldsymbol{y} \in [0,1]^s$ the kernel $K_{s,\boldsymbol{\gamma}}(\cdot, \boldsymbol{y})$ given by (25) has sufficient smoothness to lie not only in $\mathcal{W}_{s,\boldsymbol{\gamma}}^{2,2}$ but also in $\mathcal{W}_{s,\boldsymbol{\gamma}}^{\infty,1}$, thus the reproducing property of the kernel holds for all $F \in \mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ and for all q and r. Likewise $\xi_{s,N} \in \mathcal{W}_{s,\boldsymbol{\gamma}}^{\infty,1}$ and so the above equality holds for all $F \in \mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}$ for all q and r.

Introducing weights $\gamma_{\mathfrak{u}}^{1/2}$ and applying Hölder's inequality twice with conjugate pairs q, q' and r, r' in the same manner as we did in §3.1, we obtain another form of the weighted Koksma-Hlawka inequality

$$\begin{aligned} &|I_s(F) - Q_{s,N}(F)| \\ &\le \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}^{q,r}} \left(\sum_{\mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{1/2} \, \frac{\partial^{|\mathfrak{u}|} \xi_{s,N}}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r'} \right)^{1/r'} . \end{aligned}$$

It can be verified that the second factor on the right-hand side is precisely the worst-case error $e^{\mathrm{wor}}(\mathcal{P}; \mathcal{W}^{q,r}_{s,\boldsymbol{\gamma}})$, which is exactly the weighted discrepancy $D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P})$.

This approach can be useful when we are given a reproducing kernel and cannot use the Hlawka-Zaremba identity.

3.8 Relation between discrepancies with different r

We recall from (34) that for fixed $1 \le q' \le \infty$

$$D^{q',r'_1}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \ge D^{q',r'_2}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \qquad \text{for all} \qquad 1 \le r'_1 < r'_2 \le \infty\,.$$

We now provide two lemmas relating these discrepancies in other ways by modifying the weights.

The first lemma provides a result in the opposite direction to the inequality above. It allows us to use known results for $r = 1, 2$ to draw conclusions for other values of r.

Lemma 3 *Let $1 \le q' \le \infty$ and $1 \le r'_1 < r'_2 \le \infty$. Define new weights*

$$\widetilde{\gamma}_{\mathfrak{u}} := \gamma_{\mathfrak{u}}^a, \quad \mathfrak{u} \subseteq \{1:s\},$$

for arbitrary $a \in [0,1]$. Then

$$D^{q',r'_1}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \le \left(\sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\frac{(1-a)r'_1 r'_2}{2(r'_2 - r'_1)}}\right)^{\frac{r'_2 - r'_1}{r'_1 r'_2}} D^{q',r'_2}_{s,\widetilde{\boldsymbol{\gamma}}}(\mathcal{P})\,,$$

with the convention that for $r'_2 = \infty$ we have $(r'_2 - r'_1)/(r'_1 r'_2) = 1/r'_1$.

Proof: This result is proved in [17, Lemma 1] via a relationship between the corresponding norms. Here we use a similar argument to prove the result directly. We have

$$\begin{aligned} D^{q',r'_1}_{s,\boldsymbol{\gamma}}(\mathcal{P}) &= \left(\sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \left\|\gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\right\|^{r'_1}_{L^{q'}}\right)^{1/r'_1} \\ &= \left(\sum_{\emptyset \ne \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{(1-a)\,r'_1/2} \left\|\gamma_{\mathfrak{u}}^{a/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\right\|^{r'_1}_{L^{q'}}\right)^{1/r'_1} \end{aligned}$$

$$\leq \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{(1-a)\, r_1' t/2} \right)^{1/(r_1' t)} \times \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{a/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r_2'} \right)^{1/r_2'},$$

where we applied Hölder's inequality with t being the Hölder conjugate of r_2'/r_1', that is, $t = 1/(1 - r_1'/r_2') = r_2'/(r_2' - r_1')$. ♠

The second lemma allows us to trade a lower convergence rate for the discrepancy in return for less restrictive conditions on the weights.

Lemma 4 *Let $1 \leq q' \leq \infty$ and $1 \leq r_1' \leq r_2' < \infty$. Define new weights*

$$\widetilde{\gamma}_{\mathfrak{u}} := \gamma_{\mathfrak{u}}^{r_2'/r_1'}.$$

Then

$$D_{s,\boldsymbol{\gamma}}^{q',r_2'}(\mathcal{P}) \leq \left[D_{s,\widetilde{\boldsymbol{\gamma}}}^{q',r_1'}(\mathcal{P}) \right]^{r_1'/r_2'}.$$

Proof: This result is proved in [19, Lemma 1] for a special discrepancy, but the same argument holds here. We have

$$D_{s,\boldsymbol{\gamma}}^{q',r_2'}(\mathcal{P}) = \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \left\| \gamma_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r_2'} \right)^{1/r_2'}$$

$$\leq \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \left\| \widetilde{\gamma}_{\mathfrak{u}}^{1/2} \mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1) \right\|_{L^{q'}}^{r_1'} \right)^{1/r_2'} = \left[D_{s,\widetilde{\boldsymbol{\gamma}}}^{q',r_1'}(\mathcal{P}) \right]^{r_1'/r_2'},$$

where we used the estimate $\|\mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\|_{L^{q'}}^{r_2'/r_1'} \leq \|\mathrm{discr}_{\mathcal{P}}(\boldsymbol{y}_{\mathfrak{u}}, 1)\|_{L^{q'}}$, following from the fact that $r_2'/r_1' \geq 1$ and $|\mathrm{discr}_{\mathcal{P}}(\boldsymbol{y})| \leq 1$ for all $\boldsymbol{y} \in [0,1]^s$. ♠

3.9 Tractability

Tractability of multivariate problems has attracted much attention recently. For the full story see the books by Novak and Woźniakowski [40, 41]. Here we only briefly discuss the general concept.

Roughly speaking, the integration problem is *tractable* in a function space if there exists a quadrature rule whose worst-case error is bounded *polynomially in N^{-1} and s*, with an implied constant that is independent of both N and s; it is said to be *strongly tractable* if the bound is *independent of s*.

Tractability for the standard setting, i.e., the Hilbert space $\mathcal{W}^{2,2}_{s,\boldsymbol{\gamma}} = \mathcal{H}_{s,\boldsymbol{\gamma}}$ with product weights, was analyzed in [39]: it was proved there, for all possible algorithms that make use of at most N point evaluations of F, that (10) is a *necessary and sufficient condition* on the weights to achieve strong tractability.

For the Banach spaces $\mathcal{W}^{q,r}_{s,\boldsymbol{\gamma}}$ with product weights, it was proved in a series of related papers [16, 17, 18, 19] (for QMC algorithms only) that a necessary and sufficient condition for strong tractability is essentially

$$\sum_{j=1}^{\infty} \gamma_j^{r'/2} < \infty\,. \tag{35}$$

(There are some exceptions: the necessity of condition (35) for $q = 1$ does not seem to be known, and for $q < 2$ the exponent $r'/2$ in the sufficiency of condition (35) should be replaced by $r'/2 - \delta$ for $\delta > 0$ arbitrarily small.) The main observation here is that the *tractability conditions are determined by the value of r alone*. This is another supporting reason for decoupling q and r.

Note that the sufficiency of condition (35) was obtained in [17] by relating all discrepancies to $D^{\infty,\infty}_{s,\boldsymbol{\gamma}}(\mathcal{P})$ or $D^{2,2}_{s,\boldsymbol{\gamma}}(\mathcal{P})$ using Lemma 3, and then applying non-constructive results. Constructive results generally require stronger assumptions on the weights; we will discuss these in §4.

3.10 Infinite dimensional integration

Integration in the infinite dimensional setting has been analyzed in a number of recent papers, see, e.g., [38, 34, 15, 44, 10], mostly in a Hilbert space setting. In a formal sense there is little difficulty in considering integration with an infinite number of variables, in that for a function F of infinitely many variables $\boldsymbol{y} = (y_1, y_2, \ldots)$, we define the integral of F as

$$I(F) = \lim_{s\to\infty} \int_{[0,1]^s} F(y_1, \ldots, y_s, a, a, \ldots)\,\mathrm{d}(y_1, \ldots, y_s)\,,$$

whenever this limit exists, for some fixed anchor $a \in [0, 1]$. Moreover, the QMC approximation is always applied to $F(y_1, \ldots, y_s, a, a, \ldots)$ for a suitable s, thus we only ever need to evaluate functions with a finite number of variables different from the anchor a. But an additional level of error analysis

is needed to handle the truncation to a finite number of variables different from a, and a new question presents itself, namely how should the cost of evaluating $F(y_1, \ldots, y_s, a, a, \ldots)$ depend on s? The papers cited above have obtained results relating to the last question under various hypotheses, with the only common agreement being that the cost should increase with s. The model should of course depend on the problem at hand.

Note that the probabilistic example in §1.5 has a natural extension to infinite dimensions: all we need to do is to let the sum in (17) go from 1 to ∞ instead of from 1 to s. The problem considered in that section is then obtained by choosing the anchor to be $a = 0$ and setting all variables y_j with $j \geq s+1$ to have the value 0, and the infinite dimensional version corresponds to letting $s \to \infty$.

4 Constructive QMC methods

4.1 CBC construction of lattice rules based on "shift-averaged" worst-case error

Here we describe the construction of randomly shifted lattice rules in the Hilbert space $\mathcal{W}^{2,2}_{s,\boldsymbol{\gamma}}$. We denote by $D^{2,2}_{s,\boldsymbol{\gamma}}(\boldsymbol{z}, \boldsymbol{\Delta})$ the worst-case error (or discrepancy) of a shifted lattice rule in $\mathcal{W}^{2,2}_{s,\boldsymbol{\gamma}}$; an explicit formula can be obtained from (33). Since we will use random shifts, the criterion we use for the CBC construction of the generating vector $\boldsymbol{z}$ is the *shift-averaged worst-case error* $e_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ defined by

$$e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) := \int_{\boldsymbol{\Delta}\in[0,1]^s} [D^{2,2}_{s,\boldsymbol{\gamma}}(\boldsymbol{z}, \boldsymbol{\Delta})]^2 \, \mathrm{d}\boldsymbol{\Delta} \, .$$

Using term-by-term integration of (33) it can be shown that

$$e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \left(\frac{1}{N} \sum_{k=0}^{N-1} \prod_{j \in \mathfrak{u}} \left[B_2\left(\left\{ \frac{k z_j}{N} \right\} \right) + m \right] - m^{|\mathfrak{u}|} \right), \qquad (36)$$

where the braces again indicate taking the fractional part of a real number, while $B_2(x) := x^2 - x + 1/6$ is the Bernoulli polynomial of degree 2, and $m = 1/3$ in the current space with anchor 1. In general, $m = a^2 - a + 1/3$ for a general anchor a, and $m = 0$ for the unanchored variant. (Note the sum now runs from 0 to $N-1$, which is allowable because the $k = 0$ and $k = N$ terms are equal.)

Starting with $z_1 = 1$, for each $d = 2, 3, \ldots, s$ the CBC algorithm chooses z_d to be the value from set $U_N := \{1 \leq u \leq N-1 : \gcd(u, N) = 1\}$

that minimizes $e^2_{N,d,\boldsymbol{\gamma}}(z_1,\ldots,z_{d-1},z_d)$, with the previously chosen components $z_1,\ldots,z_{d-1}$ held fixed. The total number of choices in each dimension is given by the Euler totient function

$$\phi(N) = |U_N| = |\{1 \le u \le N-1 : \gcd(u,N) = 1\}|\,. \tag{37}$$

The computational cost for the CBC construction with general weights is exponential in s, but it can be as low as $\mathcal{O}(s\,N\ln N)$ operations for some special forms of weights including POD weights; this will be discussed in §5. The following theorem provides the theoretical justification for the CBC construction.

Theorem 5 *The generating vector $\boldsymbol{z}$ constructed by the CBC algorithm, minimizing $e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ in each step, satisfies for any $\lambda \in (1/2,1]$*

$$e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \left(\sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda}\,(\rho(\lambda))^{|\mathfrak{u}|}\right)^{1/\lambda} [\phi(N)]^{-1/\lambda}\,.$$

with

$$\rho(\lambda) := \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} + m^{\lambda}\,,$$

where $\zeta(x)$ is the Riemann zeta function as in §1.5, and $\phi(N)$ is the totient function given by (37)*.*

Proof: This result is partially derived in [52, Theorem 3(A)] for prime N by exploiting the connection between the Sobolev and Korobov spaces. Rather than building on the derivation of [52], here we provide a direct proof, for general N.

The Bernoulli polynomial has the expansion $B_2(x) = \sum_{h\ne0} e^{2\pi i h x}/(2\pi^2 h^2)$. Thus the constant m inside the product in (36) can be interpreted as the $h = 0$ term. A crucial technical step if an argument later in this proof is to work is to remove this $h = 0$ term from the product. We proceed as follows. Writing $b_j := B_2(\{kz_j/N\})$ and adopting the convention that an empty product is 1, we have

$$\begin{aligned} e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) &= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}\prod_{j\in\mathfrak{u}}(b_j+m) - \sum_{\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}m^{|\mathfrak{u}|} \\ &= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}\sum_{\mathfrak{v}\subseteq\mathfrak{u}} m^{|\mathfrak{u}|-|\mathfrak{v}|}\prod_{j\in\mathfrak{v}} b_j - \sum_{\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}m^{|\mathfrak{u}|} \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\mathfrak{v}\subseteq\{1:s\}}\sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}m^{|\mathfrak{u}|-|\mathfrak{v}|}\prod_{j\in\mathfrak{v}}b_j - \sum_{\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}m^{|\mathfrak{u}|}\\
&= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\mathfrak{v}\subseteq\{1:s\}}\tilde{\gamma}_{\mathfrak{v}}\prod_{j\in\mathfrak{v}}b_j - \tilde{\gamma}_{\emptyset}\\
&= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}}\tilde{\gamma}_{\mathfrak{v}}\left(\frac{1}{N}\sum_{k=0}^{N-1}\prod_{j\in\mathfrak{v}}b_j\right),
\end{aligned}
$$

where we introduced auxiliary weights defined by

$$
\tilde{\gamma}_{\mathfrak{v}} := \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}\, m^{|\mathfrak{u}|-|\mathfrak{v}|}, \quad \mathfrak{v}\subseteq\{1:s\}. \tag{38}
$$

Next we prove that the CBC construction yields

$$
e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \left(\sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}}\tilde{\gamma}_{\mathfrak{v}}^{\lambda}\left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{v}|}\right)^{1/\lambda}[\phi(N)]^{-1/\lambda} \tag{39}
$$

for all $\lambda\in(1/2,1]$. This can be proved by induction on s. The base step $s=1$ is straightforward to verify, and we omit the details here. Assume now that we have chosen the first $s-1$ components $z_1,\ldots,z_{s-1}$ and that (39) holds with s replaced by $s-1$. Using the expansion of B_2 and the "character property" of lattice rules (namely, that $\frac{1}{N}\sum_{k=0}^{N-1}e^{2\pi\mathrm{i}k\boldsymbol{h}\cdot\boldsymbol{z}/N}$ is 1 if $\boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod N$ and 0 otherwise), we can write

$$
\begin{aligned}
e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) &= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}}\tilde{\gamma}_{\mathfrak{v}}\left(\frac{1}{N}\sum_{k=0}^{N-1}\prod_{j\in\mathfrak{v}}\sum_{h\neq 0}\frac{e^{2\pi\mathrm{i}hkz_j/N}}{2\pi^2h^2}\right)\\
&= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}}\frac{\tilde{\gamma}_{\mathfrak{v}}}{(2\pi^2)^{|\mathfrak{v}|}}\left(\frac{1}{N}\sum_{k=0}^{N-1}\sum_{\boldsymbol{h}_{\mathfrak{v}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|}}\frac{e^{2\pi\mathrm{i}k\boldsymbol{h}_{\mathfrak{v}}\cdot\boldsymbol{z}_{\mathfrak{v}}/N}}{\prod_{j\in\mathfrak{v}}h_j^2}\right)\\
&= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}}\frac{\tilde{\gamma}_{\mathfrak{v}}}{(2\pi^2)^{|\mathfrak{v}|}}\left(\sum_{\substack{\boldsymbol{h}_{\mathfrak{v}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|}\\ \boldsymbol{h}_{\mathfrak{v}}\cdot\boldsymbol{z}_{\mathfrak{v}}\equiv 0 \pmod N}}\frac{1}{\prod_{j\in\mathfrak{v}}h_j^2}\right).
\end{aligned}
$$

Now we separate the terms depending on whether or not the element s is included in the set $\mathfrak{v}$, to obtain the recursive expression

$$
e^2_{N,s,\boldsymbol{\gamma}}(z_1,\ldots,z_{s-1},z_s) = e^2_{N,s-1,\boldsymbol{\gamma}}(z_1,\ldots,z_{s-1}) + \theta(z_s), \tag{40}
$$

where (suppressing the dependence of θ on $z_1, \ldots, z_{s-1}$)

$$\theta(z_s) := \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde{\gamma}_{\mathfrak{v}}}{(2\pi^2)^{|\mathfrak{v}|}} \left(\sum_{h_s\in\mathbb{Z}\setminus\{0\}} \frac{1}{h_s^2} \sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1} \\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\equiv -h_s z_s \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} h_j^2} \right).$$

If z_s^* denotes the value chosen by the CBC algorithm in dimension s, then (since the minimum is always smaller than or equal to the average) we have for all $\lambda \in (0,1]$ that

$$\begin{aligned}
[\theta(z_s^*)]^\lambda &\le \frac{1}{\phi(N)} \sum_{z_s\in U_N} [\theta(z_s)]^\lambda \\
&\le \frac{1}{\phi(N)} \sum_{z_s\in U_N} \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde{\gamma}_{\mathfrak{v}}^\lambda}{(2\pi^2)^{|\mathfrak{v}|\lambda}} \\
&\quad \cdot \left(\sum_{h_s\in\mathbb{Z}\setminus\{0\}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1} \\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\equiv -h_s z_s \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} |h_j|^{2\lambda}} \right),
\end{aligned}$$

where we used the inequality (sometimes mistakenly referred to as Jensen's inequality)

$$\left(\sum_k a_k\right)^\lambda \le \sum_k a_k^\lambda, \quad a_k \ge 0, \ \lambda \in (0,1]. \tag{41}$$

Next we separate the terms depending on whether or not h_s is a multiple of N, to obtain

$$\begin{aligned}
[\theta(z_s^*)]^\lambda &\le \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde{\gamma}_{\mathfrak{v}}^\lambda}{(2\pi^2)^{|\mathfrak{v}|\lambda}} \cdot \frac{2\zeta(2\lambda)}{N^{2\lambda}} \left(\sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1} \\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\equiv 0 \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} |h_j|^{2\lambda}} \right) \\
&\quad + \frac{1}{\phi(N)} \sum_{z_s\in U_N} \sum_{c=1}^{N-1} \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde{\gamma}_{\mathfrak{v}}^\lambda}{(2\pi^2)^{|\mathfrak{v}|\lambda}} \\
&\quad \cdot \left(\sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\} \\ h_s\equiv -c z_s^{-1} \pmod N}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1} \\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\equiv c \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} |h_j|^{2\lambda}} \right),
\end{aligned}$$

where z_s^{-1} denotes the multiplicative inverse of z_s in U_N, i.e., $z_s z_s^{-1} \equiv 1 \pmod N$. For fixed c satisfying $1 \le c \le N-1$, we have $\{c z_s^{-1} \pmod N : z_s \in$

$U_N\} = \{cz \pmod N : z \in U_N\}$. Let $g = \gcd(c, N)$. Then $\gcd(c/g, N/g) = 1$, and

$$\begin{aligned}
\sum_{z_s\in U_N} \sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\}\\ h_s\equiv -cz_s^{-1} \pmod N}} \frac{1}{|h_s|^{2\lambda}} &= \sum_{z\in U_N} \sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\}\\ h_s\equiv -cz \pmod N}} \frac{1}{|h_s|^{2\lambda}} \\
&= \sum_{z\in U_N} \sum_{m\in\mathbb{Z}} \frac{1}{|mN - cz|^{2\lambda}} \\
&= g^{-2\lambda} \sum_{z\in U_N} \sum_{m\in\mathbb{Z}} \frac{1}{|m(N/g) - (c/g)z|^{2\lambda}} \\
&= g^{-2\lambda} \sum_{z\in U_N} \sum_{\substack{h\in\mathbb{Z}\setminus\{0\}\\ h\equiv -(c/g)z \pmod{N/g}}} \frac{1}{|h|^{2\lambda}} \\
&\le g^{-2\lambda} g \sum_{a=1}^{N/g-1} \sum_{\substack{h\in\mathbb{Z}\setminus\{0\}\\ h\equiv a \pmod{N/g}}} \frac{1}{|h|^{2\lambda}} \\
&= g^{1-2\lambda} \cdot 2\zeta(2\lambda)\left(1 - (N/g)^{-2\lambda}\right) \\
&\le 2\zeta(2\lambda)\,,
\end{aligned}$$

with the last step following because $g \ge 1$ and $\lambda > 1/2$. The condition $\lambda > 1/2$ is needed to ensure that $\zeta(2\lambda) < \infty$. Hence we have

$$\begin{aligned}
[\theta(z_s^*)]^\lambda &\le \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde\gamma_\mathfrak{v}^\lambda}{(2\pi^2)^{|\mathfrak{v}|\lambda}} \cdot \frac{2\zeta(2\lambda)}{N^{2\lambda}} \left(\sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\equiv 0 \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} |h_j|^{2\lambda}} \right) \\
&\quad + \frac{1}{\phi(N)} \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \frac{\tilde\gamma_\mathfrak{v}^\lambda}{(2\pi^2)^{|\mathfrak{v}|\lambda}} \cdot 2\zeta(2\lambda) \left(\sum_{\substack{\boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}_{\mathfrak{v}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{s\}}\not\equiv 0 \pmod N}} \frac{1}{\prod_{j\in\mathfrak{v}\setminus\{s\}} |h_j|^{2\lambda}} \right) \\
&\le \frac{1}{\phi(N)} \sum_{s\in\mathfrak{v}\subseteq\{1:s\}} \tilde\gamma_\mathfrak{v}^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda}\right)^{|\mathfrak{v}|}.
\end{aligned}$$

This together with (40) and the induction hypothesis yield the result (39).

Finally we express the result in terms of the original weights. Writing $\alpha_\lambda := 2\zeta(2\lambda)/(2\pi^2)^\lambda$ and using (38) and (41), we have

$$\sum_{\emptyset\ne\mathfrak{v}\subseteq\{1:s\}} \tilde\gamma_\mathfrak{v}^\lambda\, \alpha_\lambda^{|\mathfrak{v}|} \le \sum_{\mathfrak{v}\subseteq\{1:s\}} \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} \gamma_\mathfrak{u}^\lambda\, m^{(|\mathfrak{u}|-|\mathfrak{v}|)\lambda}\, \alpha_\lambda^{|\mathfrak{v}|} - \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_\mathfrak{u}^\lambda\, m^{|\mathfrak{u}|\lambda}$$

$$
\begin{aligned}
&= \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \sum_{\mathfrak{v}\subseteq\mathfrak{u}} m^{(|\mathfrak{u}|-|\mathfrak{v}|)\lambda}\, \alpha_{\lambda}^{|\mathfrak{v}|} - \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda}\, m^{|\mathfrak{u}|\lambda} \\
&= \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} (\alpha_{\lambda} + m^{\lambda})^{|\mathfrak{u}|} - \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda}\, m^{|\mathfrak{u}|\lambda} \\
&\le \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} (\alpha_{\lambda} + m^{\lambda})^{|\mathfrak{u}|}\,.
\end{aligned}
$$

This completes the proof. ♠

Theorem 6 *If the weights satisfy*

$$\sum_{|\mathfrak{u}|<\infty} \gamma_{\mathfrak{u}}^{\lambda}\, (\rho(\lambda))^{|\mathfrak{u}|} \;<\; \infty \quad \textit{for some} \quad \lambda \in (1/2, 1], \tag{42}$$

or if we have product weights satisfying

$$\sum_{j=1}^{\infty} \gamma_j^{\lambda} \;<\; \infty \quad \textit{for some} \quad \lambda \in (1/2, 1], \tag{43}$$

then the randomly shifted lattice rule constructed by the CBC algorithm based on $e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ satisfies

$$\sqrt{\mathbb{E}\left[D^{2,2}_{s,\boldsymbol{\gamma}}(\boldsymbol{z},\cdot)\right]^2} \le C\,[\phi(N)]^{-1/(2\lambda)}\,,$$

where $\mathbb{E}$ denotes the expectation with respect to the random shift which is uniformly distributed over $[0,1]^s$, and C is independent of s and N but goes to infinity as $\lambda \to 1/2$.

Proof: The result for general weights follows directly from Theorem 5 and the definition of $e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$. In the case of product weights, we can write the sum in (42) as $\sum_{|\mathfrak{u}|<\infty} \gamma_{\mathfrak{u}}^{\lambda}(\rho(\lambda))^{|\mathfrak{u}|} = \prod_{j=1}^{\infty}(1+\rho(\lambda)\gamma_j^{\lambda}) = \exp(\sum_{j=1}^{\infty}\ln(1+\rho(\lambda)\gamma_j^{\lambda})$. The condition (43) is then deduced from the property that $\ln(1+x) \le x$ for all $x \ge 0$. ♠

Since for large values of N, $1/\phi(N) = \mathcal{O}(N^{-1}\ln\ln N)$, if (42) or (43) in Theorem 6 holds with λ arbitrarily close to $1/2$, then we have the convergence rate $\mathcal{O}(N^{-1+\delta})$ for arbitrary $\delta > 0$, with the implied constant approaching infinity as $\delta \to 0$.

4.2 CBC construction based on weighted R

There is another search criterion that can be used in the CBC construction of lattice rules: we shall refer to it as "weighted R", see (47) below. It arises from a discrepancy bound involving the classical star discrepancy. Joe [26] proved a bound on the weighted star discrepancy $D^{\infty,\infty}_{s,\boldsymbol{\gamma}}(\mathcal{P})$ for such a CBC construction with product weights and prime N. This was subsequently extended to general weights and/or composite N in [45, 46, 47].

The search criterion used for general weights [45, 47] has a fundamental difference from the criterion used for product weights [26, 46]. The discrepancy bounds established in [26, 46] can be applied to all discrepancies $D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P})$, but the same is *not* true for the results in [45, 47]. Moreover, the results in [45, 47] rely on a (restrictive) monotonicity assumption on the weights

$$\gamma_{\mathfrak{u}} \ge \gamma_{\mathfrak{v}} \quad \text{whenever} \quad \mathfrak{v} \subseteq \mathfrak{u}\,. \tag{44}$$

In particular, this condition does *not* hold for POD weights.

Here we present a discrepancy bound for general weights, which (i) uses a direct extension of the search criterion from [26, 46] for product weights, (ii) applies to all discrepancies $D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P})$, and (iii) does *not* require the monotonicity assumption (44). The results obtained in this subsection are new.

Recall that we have for all $q', r' \ge 1$

$$D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \le D^{\infty,1}_{s,\boldsymbol{\gamma}}(\mathcal{P}) = \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}[D^*(\mathcal{P}_{\mathfrak{u}})]\,,$$

where $D^*(\mathcal{P}_{\mathfrak{u}})$ is the classical star discrepancy of $\mathcal{P}_{\mathfrak{u}}$, the projection of the point set $\mathcal{P}$ in the coordinates $\boldsymbol{y}_{\mathfrak{u}}$. When $\mathcal{P}$ is a lattice rule with generating vector $\boldsymbol{z}$, it follows from [36, Theorem 3.10 and Theorem 5.6] that

$$D^*(\mathcal{P}_{\mathfrak{u}}) \le 1 - \left(1 - \frac{1}{N}\right)^{|\mathfrak{u}|} + \frac{R_N(\boldsymbol{z}_{\mathfrak{u}})}{2}\,,$$

where

$$R_N(\boldsymbol{z}_{\mathfrak{u}}) := \frac{1}{N}\sum_{k=0}^{N-1}\prod_{j\in\mathfrak{u}}\left(1 + \sum_{\substack{-N/2<h\le N/2\\ h\ne 0}} \frac{e^{2\pi \mathrm{i} h k z_j/N}}{|h|}\right) - 1\,. \tag{45}$$

Hence we conclude that for all $q', r' \ge 1$

$$D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \le \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}\left(1 - \left(1 - \frac{1}{N}\right)^{|\mathfrak{u}|}\right) + \frac{R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})}{2}\,, \tag{46}$$

where

$$R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) := \sum_{\emptyset\neq\mathrm{u}\subseteq\{1:s\}} \gamma_{\mathrm{u}}^{1/2} R_N(\boldsymbol{z}_{\mathrm{u}})\,. \tag{47}$$

Theorem 7 *The generating vector $\boldsymbol{z}$ constructed by the CBC algorithm, minimizing $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ in each step, satisfies*

$$R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \frac{2}{N} \sum_{\emptyset\neq\mathrm{u}\subseteq\{1:s\}} \gamma_{\mathrm{u}}^{1/2} \left(c_{\mathrm{lat}} \ln N\right)^{|\mathrm{u}|}\,,$$

where

$$c_{\mathrm{lat}} := \sup_{N\ge 2} \left\{ \frac{1}{\ln N} + 2 + \frac{2\pi^2(N-1)}{3\,\phi(N)\,\ln N} \right\}.$$

Proof: First we remark that the search criterion used in [26, 46] is precisely $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ for product weights, while the search criterion used in [45, 47] for general weights is

$$\tilde{R}_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) := \sum_{\emptyset\neq\mathrm{u}\subseteq\{1:s\}} \gamma_{\mathrm{u}}^{1/2} \tilde{R}_N(\boldsymbol{z}_{\mathrm{u}})\,,$$

where

$$\tilde{R}_N(\boldsymbol{z}_{\mathrm{u}}) := \frac{1}{N} \sum_{k=0}^{N-1} \prod_{j\in\mathrm{u}} \sum_{\substack{-N/2<h\le N/2\\ h\neq 0}} \frac{e^{2\pi \mathrm{i} h k z_j/N}}{|h|}\,. \tag{48}$$

(Remember that the weight γ_{u} in [26, 46] should be substituted by $\gamma_{\mathrm{u}}^{1/2}$ to be consistent with our notation here.) Notice that $\tilde{R}_N(\boldsymbol{z}_{\mathrm{u}})$ in (48) differs from $R_N(\boldsymbol{z}_{\mathrm{u}})$ in (45) in two places: it does not have a 1 added to the sum over h, and it does not have the -1 at the end. It was proved in [47] for general $N \ge 2$ that the CBC construction based on $\tilde{R}_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ yields

$$\tilde{R}_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \frac{2}{N} \sum_{\emptyset\neq\mathrm{u}\subseteq\{1:s\}} \gamma_{\mathrm{u}}^{1/2} \left(2\ln N + \frac{2\pi^2(N-1)}{3\,\phi(N)}\right)^{|\mathrm{u}|}\,, \tag{49}$$

and the proof did *not* require the monotonicity condition (44); the condition (44) was only used in the step for connecting the discrepancy $D_{s,\boldsymbol{\gamma}}^{\infty,\infty}(\mathcal{P})$ to $\tilde{R}_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$.

In the proof of Theorem 5 we removed the constant m from the product in the expression of $e_{N,s,\boldsymbol{\gamma}}^2(\boldsymbol{z})$ by defining a set of auxiliary weights. Here we

use the same argument to remove the constant 1 from the product in (45). We can show that

$$R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) = \tilde{R}_{N,s,\tilde{\boldsymbol{\gamma}}}(\boldsymbol{z})$$

for some auxiliary weights

$$\tilde{\gamma}_{\mathfrak{v}}^{1/2} := \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}\,, \qquad \mathfrak{v}\subseteq\{1:s\}\,.$$

Hence, the CBC construction based on $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ is identical to the CBC construction based on $\tilde{R}_{N,s,\tilde{\boldsymbol{\gamma}}}(\boldsymbol{z})$ for auxiliary weights $\tilde{\gamma}_{\mathfrak{v}}$, and the bound (49) applies, but with weights $\gamma_{\mathfrak{u}}$ replaced by $\tilde{\gamma}_{\mathfrak{v}}$. Writing $\alpha_N := 2\ln N + (2\pi^2/3)(N-1)/\phi(N)$, we have

$$\begin{aligned}\sum_{\emptyset\ne\mathfrak{v}\subseteq\{1:s\}} \tilde{\gamma}_{\mathfrak{v}}^{1/2}\alpha_N^{|\mathfrak{v}|} &= \sum_{\mathfrak{v}\subseteq\{1:s\}}\sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}\alpha_N^{|\mathfrak{v}|} - \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}\\ &= \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}(1+\alpha_N)^{|\mathfrak{u}|}\,.\end{aligned}$$

This completes the proof. ♠

We can say more about the special case of product weights. We shall need the following result which appeared in [20, 59] in a similar form. However, our choice of the parameters a and b here yields a better overall constant a^b.

Lemma 8 *Suppose that $\tau_j \ge 0$ for all $j \ge 1$ and $\sum_{j=1}^{\infty}\tau_j < \infty$. Let δ, a and b satisfy*

$$0 < \delta < \min\left(1, 2\sum_{j=1}^{\infty}\tau_j\right)\,,\ a := \frac{2}{\delta}\sum_{j=1}^{\infty}\tau_j\,,\ \sum_{j=b+1}^{\infty}\tau_j \le \frac{\delta}{2}\,.$$

Then for all $n > 0$ we have

$$\prod_{j=1}^{\infty}(1+\tau_j\ln n) \le a^b n^{\delta}.$$

Proof: For any arbitrary $a \ge 1$ and $b \ge 1$, we can write

$$\prod_{j=1}^{\infty}(1+\tau_j\ln n) \le \prod_{j=1}^{b}(a+\tau_j\ln n)\prod_{j=b+1}^{\infty}(1+\tau_j\ln n)$$

$$= a^b \prod_{j=1}^{b} \left(1 + \frac{\tau_j \ln n}{a}\right) \prod_{j=b+1}^{\infty} (1 + \tau_j \ln n)$$
$$= a^b \exp\left(\sum_{j=1}^{b} \ln\left(1 + \frac{\tau_j \ln n}{a}\right) + \sum_{j=b+1}^{\infty} \ln(1 + \tau_j \ln n)\right)$$
$$\le a^b \exp\left(\frac{\ln n}{a} \sum_{j=1}^{b} \tau_j + \ln n \sum_{j=b+1}^{\infty} \tau_j\right),$$

where we used the property $\ln(1+x) \le x$ for all $x \ge 0$. The result follows by choosing a and b as specified in the lemma. ♠

Theorem 9 *For any $\delta \in (0,1)$, if the weights satisfy*

$$\sum_{|\mathfrak{u}|<\infty} \gamma_{\mathfrak{u}}^{1/2} \left(\frac{c_{\rm lat}\,|\mathfrak{u}|}{e\,\delta}\right)^{|\mathfrak{u}|} < \infty \tag{50}$$

or if we have product weights satisfying

$$\sum_{j=1}^{\infty} \gamma_j^{1/2} \,<\, \infty\,, \tag{51}$$

then the lattice rule constructed by the CBC algorithm based on $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ satisfies, for all $q', r' \ge 1$,

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \le C\, N^{-1+\delta}\,,$$

where C is independent of s and N but depends on δ and tends to infinity as $\delta \to 0$.

Proof: It is argued in [45] that Bernoulli's inequality yields $1-(1-1/N)^{|\mathfrak{u}|} \le |\mathfrak{u}|/N$. Thus for general weights the first term on the right-hand side of (46) is bounded by

$$\sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2} \left(1 - \left(1 - \frac{1}{N}\right)^{|\mathfrak{u}|}\right) \le \frac{1}{N} \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2} |\mathfrak{u}|\,.$$

For the second term $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})/2$ on the right-hand side of (46) we use the bound in Theorem 7. It is shown in [47], and easily verified, that $N^{-\delta}\,(\ln N)^{|\mathfrak{u}|} \le (|\mathfrak{u}|/(e\,\delta))^{|\mathfrak{u}|}$, which yields

$$R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \,\le\, \frac{2}{N^{1-\delta}} \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2} \left(\frac{c_{\rm lat}|\mathfrak{u}|}{e\,\delta}\right)^{|\mathfrak{u}|}.$$

The result then follows by combining these two estimates.

For product weights, it is proved in [26] that

$$\sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{1/2}\left(1-\left(1-\frac{1}{N}\right)^{|\mathfrak{u}|}\right)$$
$$\le \frac{1}{N}\max\left(1,\sum_{j=1}^{\infty}\frac{\gamma_j^{1/2}}{1+\gamma_j^{1/2}}\right)\exp\left(\sum_{j=1}^{\infty}\gamma_j^{1/2}\right),$$

while Theorem 7 yields $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le (2/N)\prod_{j=1}^{s}(1+c_{\rm lat}\,\gamma_j^{1/2}\ln N)$. We now use Lemma 8 to conclude that

$$R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z}) \le \frac{2}{N^{1-\delta}}\left(\frac{2\,c_{\rm lat}}{\delta}\sum_{j=1}^{\infty}\gamma_j^{1/2}\right)^{b},$$

where b satisfies $c_{\rm lat}\sum_{j=b+1}^{\infty}\gamma_j^{1/2} \le \delta/2$. The result for product weights now follows by combining these two estimates. ♠

The following theorem allows us to construct a lattice rule with a lower convergence rate when the decay of weights is not sufficient fast.

Theorem 10 *For any $\delta \in (0,1)$, suppose we have general weights satisfying*

$$\sum_{|\mathfrak{u}|<\infty}\gamma_{\mathfrak{u}}^{\nu}\left(\frac{c_{\rm lat}\,|\mathfrak{u}|}{e\,\delta}\right)^{|\mathfrak{u}|} < \infty \quad \text{for some } \nu > \frac{1}{2},$$

or product weights satisfying

$$\sum_{j=1}^{\infty}\gamma_j^{\nu} < \infty \qquad \text{for some} \quad \nu > \frac{1}{2}\,. \tag{52}$$

Define new weights $\tilde{\gamma}_{\mathfrak{u}} := \gamma_{\mathfrak{u}}^{2\nu}$ for all $|\mathfrak{u}| < \infty$ in the case of general weights, or $\tilde{\gamma}_j := \gamma_j^{2\nu}$ for all $j \ge 1$ in the case of product weights. Then the lattice rule constructed by the CBC algorithm based on $R_{N,s,\tilde{\boldsymbol{\gamma}}}(\boldsymbol{z})$ with new weights $\tilde{\boldsymbol{\gamma}}$ satisfies, for all $q' \ge 1$ and $r' \ge 2\nu$,

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \le C\,N^{-1/(2\nu)+\delta},$$

where C is independent of s and N but depends on ν and on δ and tends to infinity as $\delta \to 0$.

Proof: We have $\sum_{|\mathfrak{u}|<\infty} \tilde{\gamma}_{\mathfrak{u}}^{1/2} (c_{\rm lat}\,|\mathfrak{u}|/(e\,\delta))^{|\mathfrak{u}|} < \infty$ in the case of general weights, and $\sum_{j=1}^{\infty} \tilde{\gamma}_j^{1/2} < \infty$ in the case of product weights. Using Lemma 4 with $r_2' = r' \ge 2\nu$ and $r_1' = r'/(2\nu) \ge 1$ so that $r_2'/r_1' = 2\nu$, we obtain

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \le \left[D_{s,\tilde{\boldsymbol{\gamma}}}^{q',r'/(2\nu)}(\mathcal{P})\right]^{1/(2\nu)}.$$

The proof is completed by using this bound together with Theorem 9, with $\boldsymbol{\gamma}$ replaced by $\tilde{\boldsymbol{\gamma}}$. ♠

We remark that the CBC constructions based on $e_{N,s,\boldsymbol{\gamma}}^2(\boldsymbol{z})$ and $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ can both be used in the Hilbert space setting with $q = r = 2$. We now briefly discuss their pros and cons. Firstly, to obtain close to order $1/N$ convergence in the case of product weights, both constructions require $\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty$, but if the weights satisfy a weaker condition then a slower convergence rate is obtained. Similar results hold for general weights, but the required condition on general weights for $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ appears to be tougher. Secondly, the quantity $e_{N,s,\boldsymbol{\gamma}}^2(\boldsymbol{z})$ is some average of $D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})$ over random shifts, while $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$ is part of a very loose upper bound on $D_{s,\boldsymbol{\gamma}}^{2,2}(\mathcal{P})$. Thus one might expect the quality of the lattice rule constructed from $e_{N,s,\boldsymbol{\gamma}}^2(\boldsymbol{z})$ to be better. Finally, Theorem 6 is a probabilistic result and it requires random shifts, while Theorems 9 and 10 are completely deterministic and do not require any shift (although shifts might still be used for practical error estimation).

4.3 Low-discrepancy sequences

Niederreiter [35, 36], Halton [11], and Sobol′ [55] sequences are low-discrepancy sequences in $[0,1]^s$ that can be generated explicitly, and that are extensible in both s and N. Furthermore, all projections of these sequences have good quality according to the classical star discrepancy bounds. See [27] for parameters to construct Sobol′ sequences in more than twelve thousand dimensions.

Throughout this section, let $\mathcal{P}^{\rm Nie}$, $\mathcal{P}^{\rm Hal}$, and $\mathcal{P}^{\rm Sob}$ denote Niederreiter, Halton, and Sobol′ sequences, respectively.

Theorem 11 *The first N points of the s-dimensional sequence $\mathcal{P} \in \{\mathcal{P}^{\rm Nie}, \mathcal{P}^{\rm Hal}, \mathcal{P}^{\rm Sob}\}$ satisfy, for any $q' \in [1,\infty)$ and $r' \in [1,\infty)$,*

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \le D_{s,\boldsymbol{\gamma}}^{\infty,r'}(\mathcal{P}) = \left(\sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{r'/2}\,[D^*(\mathcal{P}_{\mathfrak{u}})]^{r'}\right)^{1/r'},$$

with

$$D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Nie}) \le \frac{1}{N} \prod_{j\in\mathfrak{u}} \left(c_{\rm Nie}\, j\, \log_\kappa(j+\kappa)\, \ln(\kappa N)\right),$$

$$D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Hal}) \le \frac{1}{N} \prod_{j\in\mathfrak{u}} \left(c_{\rm Hal}\, j \log_2(j+1)\, \ln(eN)\right),$$

$$D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Sob}) \le \frac{1}{N} \prod_{j\in\mathfrak{u}} \left(c_{\rm Sob}\, j \log_2(j+1)\, \log_2\log_2(j+3)\, \ln(2N)\right),$$

where κ is the base for the Niederreiter sequence, and $c_{\rm Nie}$, $c_{\rm Hal}$, $c_{\rm Sob}$ are independent of s and N. The case $r' = \infty$ can be obtained by the obvious adjustment.

Proof: The bounds on $D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Nie})$, $D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Hal})$, $D^*(\mathcal{P}_{\mathfrak{u}}^{\rm Sob})$ were proved in [59], [20], and [59], respectively, see also [52]. ♠

Requirements on the weights are stated in the next theorem only for the simpler case of product weights. The theorem indicates that low-discrepancy sequences defined independently of weights can nevertheless adapt well to given weights. The conditions on the weights are stronger than (51) in Theorem 9, but it is not known whether or not the stronger requirements are artifacts of the method of proof.

Theorem 12 *Let $\mathcal{P} \in \{\mathcal{P}^{\rm Nie}, \mathcal{P}^{\rm Hal}, \mathcal{P}^{\rm Sob}\}$. Suppose for some $\nu \ge 1/2$ we have product weights satisfying*

$$\sum_{j=1}^{\infty} \gamma_j^\nu\, j\, \ln j < \infty \quad \textit{when} \quad \mathcal{P} \in \{\mathcal{P}^{\rm Nie}, \mathcal{P}^{\rm Hal}\}, \tag{53}$$

or

$$\sum_{j=1}^{\infty} \gamma_j^\nu\, j\, \ln j\, \ln\ln j < \infty \quad \textit{when} \quad \mathcal{P} = \mathcal{P}^{\rm Sob}, \tag{54}$$

then the first N points of the s-dimensional sequence $\mathcal{P}$ satisfy, for all $q' \ge 1$, $r' \ge 2\nu$ and any $\delta > 0$,

$$D_{s,\boldsymbol{\gamma}}^{q',r'}(\mathcal{P}) \le C\, N^{-1/(2\nu)+\delta},$$

where C is independent of s and N but depends on ν and on δ and tends to infinity as $\delta \to 0$.

Proof: For product weights and using $D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \le D^{q',1}_{s,\boldsymbol{\gamma}}(\mathcal{P})$, the discrepancy bounds in Theorem 11 lead to

$$D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}^{\rm Nie}) \le \frac{1}{N}\prod_{j=1}^{s}\Big(1+\gamma_j^{1/2} c_{\rm Nie}\, j\, \log_\kappa(j+\kappa)\, \ln(\kappa N)\Big),$$

$$D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}^{\rm Hal}) \le \frac{1}{N}\prod_{j=1}^{s}\Big(1+\gamma_j^{1/2} c_{\rm Hal}\, j \log_2(j+1)\, \ln(eN)\Big),$$

$$D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}^{\rm Sob})$$
$$\le \frac{1}{N}\prod_{j=1}^{s}\Big(1+\gamma_j^{1/2} c_{\rm Sob}\, j \log_2(j+1)\, \log_2\log_2(j+3)\, \ln(2N)\Big).$$

The result for $\nu = 1/2$ then follows from Lemma 8. This result was proved in [59] for $\mathcal{P}^{\rm Nie}$ and $\mathcal{P}^{\rm Sob}$, and in [20] for $\mathcal{P}^{\rm Hal}$; in both papers the result was formulated for $D^{2,2}_{s,\boldsymbol{\gamma}}(\mathcal{P})$.

To prove the result for $\nu > 1/2$, we define new weights $\tilde\gamma_j := \gamma_j^{2\nu}$ for all $j \ge 1$. Using Lemma 4 as in the proof of Theorem 10, we obtain $D^{q',r'}_{s,\boldsymbol{\gamma}}(\mathcal{P}) \le [D^{q',r'/(2\nu)}_{s,\tilde{\boldsymbol{\gamma}}}(\mathcal{P})]^{1/(2\nu)}$. The proof is completed by inserting the bound for $D^{q',r'/(2\nu)}_{s,\tilde{\boldsymbol{\gamma}}}(\mathcal{P})$. ♠

5 The CBC construction for POD weights

The criteria used in §4 for the two lattice CBC constructions take similar forms: see (36) in the case of $e^2_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$, and (47) and (45) in the case of $R_{N,s,\boldsymbol{\gamma}}(\boldsymbol{z})$. We now describe the fast CBC construction for the generic criterion

$$e^2_{N,s}(z_1,\ldots,z_s) := \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \left(\frac{1}{N}\sum_{k=0}^{N-1}\prod_{j\in\mathfrak{u}} \omega\left(\left\{\frac{kz_j}{N}\right\}\right)\right)$$

(in which the -1 and $-m^{|\mathfrak{u}|}$ terms have been omitted because they are independent of $\boldsymbol{z}$), with POD weights, see (16). We need only very minor modifications of the "order-dependent" case in [4, Section 4.1].

Suppose we are at the point in the CBC algorithm where we want to choose the dth component z_d. It makes sense to consider $e^2_{N,d}(z_1,\ldots,z_d) =: E^2_d(z_d)$ as a function of z_d. We can write

$$E^2_d(z_d) = \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\ell=1}^{d}\Gamma_\ell \sum_{\substack{\mathfrak{u}\subseteq\{1:d\}\\ |\mathfrak{u}|=\ell}}\prod_{j\in\mathfrak{u}}\left[\gamma_j\,\omega\left(\left\{\frac{kz_j}{N}\right\}\right)\right]$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \sum_{\ell=1}^{d} \Gamma_\ell \Bigg(\underbrace{\sum_{\substack{\mathfrak{u} \subseteq \{1:d-1\} \\ |\mathfrak{u}|=\ell}} \prod_{j \in \mathfrak{u}} \left[\gamma_j \, \omega \left(\left\{ \frac{k z_j}{N} \right\} \right) \right]}_{p_{d-1,\ell}(k)}$$

$$+ \gamma_d \, \omega \left(\left\{ \frac{k z_d}{N} \right\} \right) \underbrace{\sum_{\substack{\mathfrak{u} \subseteq \{1:d-1\} \\ |\mathfrak{u}|=\ell-1}} \prod_{j \in \mathfrak{u}} \left[\gamma_j \, \omega \left(\left\{ \frac{k z_j}{N} \right\} \right) \right]}_{p_{d-1,\ell-1}(k)} \Bigg)$$

$$= e^2_{N,d-1}(z_1, \ldots, z_{d-1})$$

$$+ \frac{\gamma_d}{N} \sum_{k=0}^{N-1} \omega \left(\left\{ \frac{k z_d}{N} \right\} \right) \left(\sum_{\ell=1}^{d} \Gamma_\ell \, p_{d-1,\ell-1}(k) \right), \tag{55}$$

with $e^2_{N,0} := 0$, and the products $p_{d,\ell}(k)$ are defined recursively by

$$p_{d,0}(k) := 1\,,$$

$$p_{d,\ell}(k) := p_{d-1,\ell}(k) \, + \, \gamma_d \, \omega \left(\left\{ \frac{k z_d}{N} \right\} \right) p_{d-1,\ell-1}(k)\,. \tag{56}$$

Let $\mathbb{Z}_N := \{0, 1, \ldots, N-1\}$ denote the set of the integers modulo N, and let $U_N := \{u \in \mathbb{Z}_N : \gcd(u, N) = 1\}$ denote the multiplicative group of integers modulo N as before, with $|U_N| = \phi(N)$. We need to evaluate $E^2_d(z_d)$ for every choice of $z_d \in U_N$, which suggests the definition of the vectors

$$\boldsymbol{E}^2_d := \left[E^2_d(z) \right]_{z \in U_N}, \quad \boldsymbol{p}_{d,\ell} := \left[p_{d,\ell}(k) \right]_{k \in \mathbb{Z}_N}, \tag{57}$$

and the matrix

$$\boldsymbol{\Omega}_N := \left[\omega \left(\left\{ \frac{kz}{N} \right\} \right) \right]_{\substack{z \in U_N \\ k \in \mathbb{Z}_N}} = \left[\omega \left(\frac{kz \bmod N}{N} \right) \right]_{\substack{z \in U_N \\ k \in \mathbb{Z}_N}}. \tag{58}$$

We now observe from (55) that the vector $\boldsymbol{E}^2_d$ can be expressed in terms of a matrix-vector product with the matrix $\boldsymbol{\Omega}_N$ as

$$\boldsymbol{E}^2_d := \mathbf{1}_{\phi(N)} \, e^2_{N,d-1}(z_1, \ldots, z_{d-1}) \, + \, \frac{\gamma_d}{N} \, \boldsymbol{\Omega}_N \left(\sum_{\ell=1}^{d} \Gamma_\ell \, \boldsymbol{p}_{d-1,\ell-1} \right)$$

where $\mathbf{1}_t$ denotes a vector of ones of length t. The CBC algorithm picks the value of $z_d \in U_N$ which corresponds to the smallest entry in $\boldsymbol{E}^2_d$. Then it is

clear from (56) that the vectors $\boldsymbol{p}_{d,\ell}$ for the next iteration can be obtained recursively via

$$\boldsymbol{p}_{d,\ell} := \boldsymbol{p}_{d-1,\ell} + \boldsymbol{\Omega}_N(z_d) \,.*\, \boldsymbol{p}_{d-1,\ell-1}$$

where $\boldsymbol{\Omega}_N(z_d)$ denotes the row of $\boldsymbol{\Omega}_N$ corresponding to the chosen z_d, and the operator $.*$ denotes the element-wise vector multiplication. Since the vectors $\boldsymbol{p}_{d-1,\ell}$ are no longer needed in the next iteration, we can simply overwrite $\boldsymbol{p}_{d-1,\ell}$ with $\boldsymbol{p}_{d,\ell}$. Hence, starting with the vectors $\boldsymbol{p}_{0,\ell} := \mathbf{1}_N$, we require only $\mathcal{O}(sN)$ storage for POD weights.

The trick now is to order the indices $z \in U_N$ and $k \in \mathbb{Z}_N$ in (57) and (58) in a clever way to allow fast matrix-vector multiplications. For this we can follow the discussion in [4, Section 4.2]; it covers prime N and the case where N is a power of a prime. In particular, the only change needed specifically for POD weights is the update step, [4, Top of page 2177],

$$\boldsymbol{p}_{d,\ell}^{\langle g^{-1}\rangle} := \Pi_{g^{-1}}^{\top} \boldsymbol{p}_{d,\ell} = \boldsymbol{p}_{d-1,\ell}^{\langle g^{-1}\rangle} + \gamma_d \, \boldsymbol{\Omega}_{p^m}^{\langle g^{-1}\rangle}(z_d) \,.*\, \boldsymbol{p}_{d-1,\ell-1}^{\langle g^{-1}\rangle} .$$

The overall CBC construction cost is then $\mathcal{O}(s\, N \ln N)$ operations.

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