Finite-order integration weights can be dangerous

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Abstract

Finite-order weights have been introduced in recent years to describe the often occurring situation that multivariate integrands can be approximated by a sum of functions each depending only on a small subset of the variables. The aim of this paper is to demonstrate the danger of relying on this structure when designing lattice integration rules, if the true integrand has components lying outside the assumed finite-order function space. It does this by proving, for weights of order two, the existence of 3-dimensional lattice integration rules for which the worst case error is of order $O(N^{-1/2})$, where N is the number of points, yet for which there exists a smooth 3-dimensional integrand for which the integration rule does not converge.

1 Introduction

Recent years have seen a rising interest in using lattice rules for the numerical integration of high-dimensional integrals over the unit cube,

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

with d in the hundreds or even thousands. The two main drivers of this developments have been, on the one hand, the demonstration by Paskov and Traub [11] that some key problems of mathematical finance can be successfully approximated by equal weight (i.e. quasi-Monte Carlo or QMC) integration rules of the form

$$Q_{d,N}f := \frac{1}{N} \sum_{j=0}^{N-1} f(\mathbf{t}^{(j)}), \qquad (1)$$

with well chosen deterministic points $\mathbf{t}^{(j)} \in [0, 1]^d$, j = 1, ..., N; and on the other hand, the development of fast component-by-component (or CBC) algorithms for the determination of good rank-1 lattice points, i.e. point sets of the form

$$\mathbf{t}^{(j)} = \left\{ j \frac{\mathbf{z}}{N} \right\}, \qquad j = 1, \dots, N, \tag{2}$$

where \mathbf{z} is a well chosen integer vector of length d, and the braces indicate that each component of $j\mathbf{z}/N$ is to be replaced by its fractional part. For an account of the recent lattice rule developments see [8]. The CBC construction of rank-1 lattice rules first appeared in [14], and the fast FFT implementation of the CBC construction in [10].

It is by now well understood that the high-dimensional integrands f that can be successfully treated in this way are rather special. In particular, their effective dimensionality is quite small: either $f(\mathbf{x}) = f(x_1, x_2, \ldots, x_d)$ depends mainly on the first few variables x_1, x_2, \ldots (in which case the "truncation dimension" is small); or f can be well approximated by a sum of functions of at most say two or three variables at a time (in which case the "superposition dimension" is small). These concepts were introduced in [1]; see that paper for a precise definition of effective dimension.

These special features of typical integrands can be modelled by introducing "weights" into the underlying function spaces. The earliest weights, in the paper [15], were of the "product" form, while a more recent way of reflecting low effective dimensionality in the superposition sense is to use "finite-order" weights, introduced in [4]; these concepts are described below. The weights then appear as parameters in the CBC algorithms.

The purpose of the present paper is to argue that the use of finite-order weights can be dangerous in applications. But before this question can be addressed, it is necessary to describe the function spaces and the role of the "weights" in more detail.

The function spaces that underlie the CBC constructions are reproducing kernel Hilbert spaces, for which in the unweighted case the kernel takes the form of a product,

$$K_d(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^d (1 + \kappa(x_i, y_i)), \qquad \mathbf{x} = (x_1, \dots, x_d), \ \mathbf{y} = (y_1, \dots, y_d),$$

where $\kappa(x, y)$ is a 1-dimensional kernel whose choice we leave free for the moment. The unweighted kernel $K_d(\mathbf{x}, \mathbf{y})$ can be rewritten as a sum over

subsets of the variables,

$$K_d(\mathbf{x}, \mathbf{y}) = \sum_{u \subseteq \{1, \dots, d\}} \prod_{i \in u} \kappa(x_i, y_i), \qquad \mathbf{x} = (x_1, \dots, x_d), \ \mathbf{y} = (y_1, \dots, y_d).$$
(3)

We let H_d denote the unweighted Hilbert space whose kernel is K_d . The corresponding "weighted" space H_d^{Γ} , in its most general form, is the reproducing kernel Hilbert space with the reproducing kernel K_d^{Γ} , given by

$$K_d^{\Gamma}(\mathbf{x}, \mathbf{y}) := \sum_{u \subseteq \{1, \dots, d\}} \Gamma_u \prod_{i \in u} \kappa(x_i, y_i), \qquad \mathbf{x} = (x_1, \dots, x_d), \ \mathbf{y} = (y_1, \dots, y_d),$$
(4)

where Γ_u , for $u \subseteq \{1, \ldots, d\}$, are prescribed non-negative "weights". The unweighted case is of course recovered by setting $\Gamma_u = 1$ for all subsets u.

In essence, the weight Γ_u reflects the relative importance in the function space H_d^{Γ} of the subset $u \subseteq \{1, \ldots, d\}$ of the variables. For the specific spaces considered here (see Section 3) it is easily seen that the space H_d^{Γ} is equivalent to H_d if $\Gamma_u > 0$ for all $u \subset \{1, \ldots, d\}$. This equivalence fails if $\Gamma_u = 0$ for some $u \subseteq \{1, \ldots, d\}$.

In (4) we allow the most general form of weights, as introduced by [6]. In practice, however, simplified models of the weights must be used, both to reduce the number of free parameters, and to make feasible the CBC construction of the integer vector \mathbf{z} in (2). In the original "product" form of weights, see [15], the Γ_u take the form

$$\Gamma_u = \prod_{i \in u} \gamma_i, \qquad u \subseteq \{1, \dots, d\} , \qquad (5)$$

where the γ_i are prescribed non-negative parameters (which are also called "weights"). In this case the reproducing kernel (4) can be written as a product,

$$K_d^{\Gamma}(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^d (1 + \gamma_i \kappa(x_i, y_i)), \qquad \mathbf{x} = (x_1, \dots, x_d), \ \mathbf{y} = (y_1, \dots, y_d).$$

The space H_d^{Γ} is then a tensor product of 1-dimensional Hilbert spaces.

The finite-order weights which are the main subject of this paper have the defining property that for some natural number q > 0 the weights vanish for |u| > q, that is

$$\Gamma_u = 0 \qquad \text{for} \quad |u| > q. \tag{6}$$

The number q in (6) is the "order" of the finite order weights. The finiteorder weights used in practice usually have a further drastic simplification, see [4] Section 6, namely that the weight Γ_u depends on u only through its cardinality, that is

$$\Gamma_u = \Gamma_{|u|}, \qquad 1 \le |u| \le q.$$

Because the superposition dimension for some financial problems is approximately 2 (see [17]), it has sometimes been suggested that weights of order 2 (i.e. with q = 2 in (6)) might be used in the construction of practical lattice rules for such problems. Of course the order-2 weights are indeed suitable if the integrand is exactly expressible in the form

$$f(\mathbf{x}) = f(x_1 \dots, x_d) = \sum_{1 \le i < j \le d} f_{ij}(x_i, x_j) , \qquad (7)$$

that is, if f is a sum of functions of at most two variables at a time. In real applications, however, f will also contain (possibly small) components that cannot be expressed in this form. The underlying hope of those (including this author) who have advocated order-2 weights has been that such functions, even though not strictly covered, will nevertheless be integrated well enough by lattice rules constructed with order-2 weights. We shall argue in this paper that this hope is forlorn.

By definition, the "worst-case error" of the QMC rule (1) is

$$e_{d,N}^{\Gamma}(Q_{d,N}) := \sup\{|Q_{d,N}f - I_df| : \|f\|_{H_d^{\Gamma}} \le 1\}.$$
(8)

The nature of the CBC algorithm for the lattice rule with points given by (2) is that it successively chooses the components z_1, z_2, \ldots, z_d of the vector \mathbf{z} in such a way as to minimize $e_{s,N}^{\Gamma}(Q_{s,N})$ for $s = 1, \ldots, d$, where $Q_{s,N}$ denotes the *s*-dimensional lattice rule generated by z_1, \ldots, z_s . It is a "greedy" algorithm, in that once a component z_s is determined it is never changed.

It was shown in [14], for the particular case of the unweighted "Korobov" space, that the worst case error of the corresponding CBC rules have an order of convergence of $O(N^{-1/2})$. By now similar results are known for product weights in Korobov and Sobolev spaces, and it is even known, (see [7, 2]) that the convergence order for the case of product weights and Sobolev spaces can be improved to $O(N^{-1+\delta})$ for arbitrary $\delta > 0$, with the implied constant depending on δ . (Much of the recent interest has been on the *d*-dependence of the constants, but that is not our concern here.)

Now we come to the central thesis of this paper, which is that CBC rules constructed with finite-order weights can be dangerously unreliable in practical situations. Suppose we take as our integrand an arbitrary function $f \in H_d$. In the case of product weights, provided that (as usual) we take all weights positive, i.e. $\gamma_j > 0$ for all $j \ge 0$, a function f in H_d also belongs to H_d^{Γ} , albeit with a different norm. That means that $Q_{d,n}f - I_df$ automatically converges with the same $O(N^{-1+\delta})$ rate of convergence as $e_{d,n}^{\Gamma}$, since from (8)

$$|Q_{d,n}f - I_d f| \le e_{d,n}^{\Gamma}(Q_{d,N}) ||f||_{H_{4}^{\Gamma}}$$

The situation with finite-order weights Γ is very different. Formally, the problem is that an arbitrary $f \in H_d$ does **not** in general lie in H_d^{Γ} . More pointedly, we shall show that rules that perform well for $f \in H_d^{\Gamma}$ need not converge at all for $f \in H_d \setminus H_d^{\Gamma}$.

The problem arises even for very small values of d, even d = 3. We shall show in Section 4 that for weights of order 2 there exist sequences of 3-dimensional lattice rules $Q_{3,N}$ for which $e_{3,N}^{\Gamma}(Q_{3,N}) \leq c/\sqrt{N}$, yet which converge to the wrong answer for some $f \in H_3$.

In this way we are able to demonstrate that, for the case of finite-order weights, small values of the worst-case error do not guarantee convergence for an integrand in H_d but not in H_d^{Γ} . Since the CBC algorithm relies entirely on minimising the worst-case error, we conclude that the general use of finite-order weights cannot be recommended.

In Section 2 we introduce some machinery ("u-discrepancies") that will assist us when looking at different choices of weights (the u-discrepancies having the advantage of being independent of weights). In Section 3 we specialise to two choices of function space, one a Korobov space of periodic functions with square integrable mixed first derivatives, the other a Sobolev space of non-periodic functions with square integrable mixed first derivatives. In Section 4 we state the main results of the paper, Theorems 4.1 and 4.2. The theorems are proved in Sections 5 and 6. A final discussion in Section 7 considers the implications for integrals in higher dimensions.

2 Worst-case errors and *u*-discrepancies

For the point set of the QMC rule (1) we use the notation

$$T_N := {\mathbf{t}^{(0)}, \dots, \mathbf{t}^{(N-1)}} \subseteq [0, 1]^d.$$

In a reproducing kernel Hilbert space H_d with reproducing kernel K_d it is well known that the squared worst-case error $e_{d,N}(T_N)$ for the QMC rule can be written as

$$e_{d,N}(T_N)^2 = \int_{[0,1]^{2d}} K_d(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$
$$- 2 \int_{[0,1]^d} \frac{1}{N} \sum_{j=0}^{N-1} K_d(\mathbf{x}, \mathbf{t}^{(j)}) d\mathbf{x} + \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} K_d(\mathbf{t}^{(j)}, \mathbf{t}^{(\ell)}).$$
(9)

It follows that for the weighted space H_d^{Γ} with kernel K_d^{Γ} given by (4) we can write the squared worst-case error as the sum

$$e_{d,N}^{\Gamma}(T_N)^2 = \sum_{\emptyset \neq u \subseteq \{1,...,d\}} \Gamma_u D_u(T_N)^2 , \qquad (10)$$

where $D_u(T_N)$ (which we shall call the "u-discrepancy" of the point set T_N) is given by

$$D_{u}(T_{N})^{2} := \int_{[0,1]^{2|u|}} k_{u}(\mathbf{x}_{u}, \mathbf{y}_{u}) d\mathbf{x}_{u} d\mathbf{y}_{u}$$
$$- 2 \int_{[0,1]^{|u|}} \frac{1}{N} \sum_{j=1}^{N} k_{u}(\mathbf{x}_{u}, \mathbf{t}_{u}^{(j)}) d\mathbf{x}_{u} + \frac{1}{N^{2}} \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} k_{u}(\mathbf{t}_{u}^{(j)}, \mathbf{t}_{u}^{(\ell)}), \quad (11)$$

and where for a given vector $\mathbf{x} \in [0, 1]^d$ we use the notation \mathbf{x}_u for the |u|-dimensional vector with components x_i for $i \in u$, and

$$k_u(\mathbf{x}_u, \mathbf{y}_u) := \prod_{i \in u} \kappa(x_i, y_i), \quad \emptyset \neq u \subseteq \{1, \dots, d\}.$$

The *u*-discrepancies $D_u(T_N)$ have been discussed in [5, 18]. A useful feature of these quantities is that they are independent of the weights Γ_u .

For the particular case of weights of finite order q, we note that (10) can be written as

$$e_{d,N}^{\Gamma}(T_N)^2 = \sum_{\substack{u \subseteq \{1,\dots,d\}, \\ 0 < |u| \le q}} \Gamma_u D_u(T_N)^2.$$
(12)

The worst-case error $e_{d,N}^{\Gamma}(T_N)$ now depends only on the projections of the point set T_N which involve at most q components at a time. Thus if q = 2 then the progress of the CBC algorithm is completely unaffected by the quality of 3-dimensional projections or higher.

3 Specific function spaces

In this section we specialise the choice of reproducing kernel, so that we may later state precise convergence results.

We consider here two commonly used function spaces: first, a Korobov space, in which the functions are 1-periodic with respect to each variable; and second, a non-periodic Sobolev space. In both cases the elements of the space have square-integrable mixed first derivatives. In the second case we extend the lattice rule by allowing a shift $\Delta \in [0, 1]^d$; that is, our rule is now the shifted lattice rule

$$Q_{d,N}(\mathbf{z}, \mathbf{\Delta})f := \frac{1}{N} \sum_{j=0}^{N-1} f\left(\left\{j\frac{\mathbf{z}}{N} + \mathbf{\Delta}\right\}\right).$$
(13)

In the Korobov case we take the 1-dimensional kernel $\kappa(x, y)$ in (4) to be given by

$$\kappa(x,y) := \frac{1}{2\pi^2} \sum_{h \neq 0} \frac{e^{2\pi i h(x-y)}}{h^2}$$

$$= B_2(\{x-y\}), \qquad x, y \in [0,1],$$
(14)

where B_2 is the Bernoulli polynomial of degree 2,

$$B_2(x) := x^2 - x + \frac{1}{6}.$$

(More general Korobov spaces, with the exponent of h, instead of being 2, replaced by α with $\alpha > 1$, are often considered. For the present purposes the case $\alpha = 2$ suffices.) We note that the normalisation constant $(2\pi^2)^{-1}$ in (14) is unconventional; it is introduced here to simplify the subsequent relationship with Sobolev spaces.

The inner product in the unweighted 1-dimensional Korobov space H_1 is

$$(f,g)_{H_1} := \hat{f}(0)\overline{\hat{g}(0)} + 2\pi^2 \sum_{h \neq 0} h^2 \hat{f}(h)\overline{\hat{g}(h)},$$

where

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

This ensures that the reproducing property,

$$(f, K_1(\cdot, y))_{H_1} = \hat{f}(0) + \sum_{h \neq 0} \hat{f}(h) e^{2\pi i h y} = f(y),$$

for all $f \in H_1$. This inner product may be written in terms of derivatives of f and g as

$$(f,g)_{H_1} = \int_0^1 f(x) \mathrm{d}x \overline{\int_0^1 g(x) \mathrm{d}x} + \frac{1}{2} \int_0^1 f'(x) \overline{g'(x)} \mathrm{d}x.$$

Thus H_1 contains the absolutely continuous 1-periodic functions on [0, 1] whose first derivatives are in $L_2(0, 1)$. Similarly, since the unweighted space H_d is a tensor product space, it contains all 1-periodic functions on $[0, 1]^d$ whose mixed first derivatives are square integrable on $[0, 1]^d$.

In this Korobov case (because $\int_0^1 \kappa(x, y) dy = 0 \ \forall x$) the expression (11) for the squared *u*-discrepancy simplifies to

$$D_u(T_N)^2 = \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} \prod_{i \in u} B_2(\{t_i^{(j)} - t_i^{(\ell)}\}), \quad \emptyset \neq u \subseteq \{1, \dots, d\}.$$

When the integration points are given by the lattice formula (2) with generating vector \mathbf{z} the last formula simplifies to a single sum,

$$D_{|u|,N}(\mathbf{z}_u)^2 = \frac{1}{N} \sum_{j=0}^{N-1} \prod_{i \in u} B_2\left(\left\{\frac{jz_i}{N}\right\}\right) .$$
(15)

Note that for this lattice-rule case we use in (15) a different notation for the u-discrepancy on the left side, as the discrepancy depends only on N and the cardinality |u| of the set u, and on the components z_j of \mathbf{z} for which $j \in u$.

In the unweighted Korobov space H_d the worst-case error corresponding to (15) is given by, using (10) with $\Gamma_u = 1$ for all u, and again using a special notation for this lattice rule case,

$$e_{d,N}(\mathbf{z})^2 = \frac{1}{N} \sum_{j=0}^{N-1} \prod_{i=1}^d \left(1 + B_2\left(\left\{\frac{jz_i}{N}\right\}\right) \right) - 1,$$
(16)

a formula which we shall find useful later.

The second space we consider is sometimes called the "unanchored" Sobolev space. (See [16] for a detailed discussion.) In this case the 1-dimensional kernel takes the form

$$\kappa(x,y) = \frac{1}{2}B_2(\{x-y\}) + \left(x-\frac{1}{2}\right)\left(y-\frac{1}{2}\right), \ x,y \in [0,1),$$

while the corresponding inner product is for real functions f, g

$$(f,g)_{H_1} = \int_0^1 f(x) \mathrm{d}x \int_0^1 g(x) \mathrm{d}x + \int_0^1 f'(x)g'(x) \mathrm{d}x.$$

The *u*-discrepancy for the Sobolev space is

$$D_u(T_N)^2 = \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} \prod_{i \in u} \left(\frac{1}{2} B_2(\{t_i^{(j)} - t_i^{(\ell)}\}) + \left(t_i^{(j)} - \frac{1}{2}\right) \left(t_i^{(\ell)} - \frac{1}{2}\right) \right) .$$

In the case of the shifted lattice rule (13) (and again introducing an obvious notation) this becomes

$$D_{|u|,N}(\mathbf{z}_{\mathbf{u}}, \boldsymbol{\Delta}_{\mathbf{u}})^{2} = \frac{1}{N^{2}} \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} \prod_{i \in u} \left(\frac{1}{2} B_{2} \left(\left\{ \frac{(j-\ell)z_{i}}{N} \right\} \right) \right) + \left(\left\{ \frac{jz_{i}}{N} + \Delta_{i} \right\} - \frac{1}{2} \right) \left(\left\{ \frac{\ell z_{i}}{N} + \Delta_{i} \right\} - \frac{1}{2} \right). \quad (17)$$

It is well known that the Sobolev space result simplifies dramatically if, as in [12], we treat the components of the shift $\boldsymbol{\Delta}$ as random variables uniformly distributed on $[0, 1]^d$. In that case it is appropriate to consider, instead of the worst-case error $e_{d,N}^{\Gamma}(\mathbf{z}, \boldsymbol{\Delta}) := e_{d,N}^{\Gamma}(T_N(\mathbf{z}, \boldsymbol{\Delta}))$ the shift-averaged worst-case error

$$e_{d,N}^{\Gamma,\mathrm{sh}}(\mathbf{z}) := \left(\int_{[0,1]^d} e_{d,N}^{\Gamma}(\mathbf{z}, \mathbf{\Delta})^2 \mathrm{d}\mathbf{\Delta}
ight)^{1/2}.$$

Replacing (10) we then have

$$e_{d,N}^{\Gamma,\mathrm{sh}}(\mathbf{z})^2 = \sum_{\emptyset \neq u \subseteq \{1,\dots,d\}} \Gamma_u D_{|u|,N}^{\mathrm{sh}}(\mathbf{z}_u)^2 ,$$

where $D_{|u|,N}^{\rm sh}$ denotes the shift-averaged *u*-discrepancy defined by

$$D_{|u|,N}^{\mathrm{sh}}(\mathbf{z}_u)^2 := \int_{[0,1]^{|u|}} D_{|u|,N}(\mathbf{z}_u, \boldsymbol{\Delta}_u)^2 \mathrm{d}\boldsymbol{\Delta}_u$$
$$= \frac{1}{N} \sum_{j=0}^{N-1} \prod_{i \in u} B_2\left(\left\{\frac{jz_i}{N}\right\}\right),$$

which is exactly the same as the Korobov u-discrepancy given by (15). This well known connection between the Sobolev and Korobov cases allows us to consider the Korobov and Sobolev cases at the same time.

Thus we now let $e_{d,N}^{\Gamma}(\mathbf{z})$ denote the worst-case error for the *N*-point lattice rule with vector $\mathbf{z} \in \{0, 1, \dots, N-1\}^d$ in the Korobov case, or the root mean square worst-case error (averaged over shifts) in the Sobolev case. Then we have

$$e_{d,N}^{\Gamma}(\mathbf{z})^2 = \sum_{\emptyset \neq u \subseteq \{1,\dots,d\}} \Gamma_u D_{|u|,N}(\mathbf{z}_u)^2 , \qquad (18)$$

with $D_{|u|,N}(\mathbf{z}_u)$ given by (15). We shall for simplicity assume from now on that N is prime. Then with $\mathbb{Z}_N^+ := \{1, \ldots, N-1\}$, we denote the root-mean-square average over \mathbf{z} of $e_{d,N}^{\Gamma}(\mathbf{z})$ by $M_{d,N}^{\Gamma}$; that is

$$\left(M_{d,N}^{\Gamma}\right)^{2} := \frac{1}{(N-1)^{d}} \sum_{\mathbf{z} \in (\mathbb{Z}_{N}^{+})^{d}} e_{d,N}^{\Gamma}(\mathbf{z})^{2}.$$

The evaluation of averages of this kind traces back at least to Korobov in the 1950s.

For the unweighted case, starting from (16), or using [4], Theorem 1, we find explicitly

$$M_{d,N}^{2} = -1 + \frac{1}{N} \left(\frac{7}{6}\right)^{d} + \frac{N-1}{N} \left(1 - \frac{1}{6N}\right)^{d} \\ \leq \frac{1}{N} \left(\frac{7}{6}\right)^{d}.$$
(19)

4 The danger of finite-order weights

In this section we restrict attention to weights of finite order 2, i.e.

 $\Gamma_u = 0$ for |u| > 2, $u \subseteq \{1, \dots, d\}$.

The following theorems show that weights of order 2 can give wrong answers even for d = 3. While we have limited the statements to d = 3 and weights of order 2, it seems reasonable to suppose that the problem here revealed will not be solved by going to finite-order weights of higher order or higher values of d. The first theorem is for the case of weighted Korobov spaces, the second for weighted Sobolev spaces.

Theorem 4.1 Let d = 3 and take the space H_3^{Γ} to be a weighted Korobov space of order 2, i.e. $\Gamma_{\{1,2,3\}} = 0$, and H_3 to be the unweighted Korobov space. Let N be prime. Then there exists $\mathbf{z} \in \{1, \dots, N-1\}^3$ such that the worst-case error in H_3^{Γ} satisfies

$$e_{3,N}^{\Gamma}(\mathbf{z}) \le \frac{c_{\Gamma}}{\sqrt{N}} \tag{20}$$

for some c_{Γ} independent of N, yet such that for some $g \in H_3$ the lattice rule $Q_{3,N}(\mathbf{z})g$ does not converge to the exact integral I_3g .

Theorem 4.2 Let d = 3 and take the space H_3^{Γ} to be a weighted Sobolev space of order 2, i.e. $\Gamma_{\{1,2,3\}} = 0$, and H_3 to be the unweighted Sobolev space. Let N be prime. Then there exists $\mathbf{z} \in \{1, \dots, N-1\}^3$ such that the shift-averaged worst-case error in H_3^{Γ} satisfies

$$e_{3,N}^{\Gamma,\mathrm{sh}}(\mathbf{z}) \le \frac{c_{\Gamma}}{\sqrt{N}}$$
(21)

for some c_{Γ} independent of N, yet such that for some $g \in H_3$ the meansquare expected error $\mathbb{E}[(Q_{3,N}(\mathbf{z}, \boldsymbol{\Delta})g - I_3g)^2]$ of the randomly shifted lattice rule $Q_{3,N}(\mathbf{z}, \boldsymbol{\Delta})g$ does not converge to zero.

The proofs are given in the next sections. In the remainder of this section we discuss the implications of the results.

A 3-dimensional lattice rule $Q_{3,N}(\mathbf{z})$ automatically generates three 2dimensional lattice rules and three 1-dimensional lattice rules, simply by omitting one or two of the variables. The rules so obtained are referred to as "projections" of the original rule. The 2-dimensional projections onto the xy, xz, and yz planes, respectively, are the N-point lattice rules (possibly with not all points distinct) generated by $(z_1, z_2), (z_1, z_3)$ and (z_2, z_3) respectively. Similarly, the three 1-dimensional projections onto the x, y, zaxes are the N-point rules generated by z_1, z_2, z_3 respectively. The quality of the projections of the rule $Q_{3,N}(\mathbf{z})$ onto the subspace corresponding to the non-empty subsets $u \subseteq \{1, 2, 3\}$ of the variables may be measured by the corresponding *u*-discrepancies $D_{|u|,N}(\mathbf{z}) = D_{|u|,N}(\mathbf{z}_u)$.

The worst-case error $e_{3,N}^{\Gamma}(\mathbf{z})$ (or the shift-averaged worst-case error $e_{3,N}^{\Gamma,\text{sh}}(\mathbf{z})$ in the Sobolev case) for general weights Γ depends on the quality of all seven of the projections corresponding to the non-empty subsets of $\{1, 2, 3\}$, since (18) gives for d = 3

$$e_{3,N}^{\Gamma}(\mathbf{z})^2 = \sum_{\emptyset \neq u \subseteq \{1,2,3\}} \Gamma_u D_{|u|,N}(\mathbf{z}_u)^2.$$
(22)

For the case specified in the theorems, with $\Gamma_{\{1,2,3\}} = 0$, this reduces to

$$e_{3,N}^{\Gamma}(\mathbf{z})^{2} = \Gamma_{\{1\}} D_{1,N}(z_{1})^{2} + \Gamma_{\{2\}} D_{1,N}(z_{2})^{2} + \Gamma_{\{3\}} D_{1,N}(z_{3})^{2} + \Gamma_{\{1,2\}} D_{2,N}(z_{1},z_{2})^{2} + \Gamma_{\{2,3\}} D_{2,N}(z_{2},z_{3})^{2} + \Gamma_{\{1,3\}} D_{2,N}(z_{1},z_{3})^{2}.$$
(23)

Thus for the theorem to hold for general weights Γ_u with $|u| \leq 2$ we must have

$$D_{|u|,N}(\mathbf{z}_u) \le \frac{c}{\sqrt{N}} \quad \forall \ u \subseteq \{1,2,3\}, \ 0 < |u| \le 2,$$
 (24)

for some c > 0. That is, every 1-dimensional and 2-dimensional projection of $Q_{3,N}(\mathbf{z})$ must be a "good" rule, in the sense of (24). Yet from the last part of the theorem we must have, for the 3-dimensional discrepancy,

$$D_{3,N}(\mathbf{z}) \not\to 0$$
 as $N \to \infty$.

For suppose the contrary, that $D_{3,N}(\mathbf{z}) \to 0$ as $N \to \infty$. Then even in the unweighted case (i.e. $\Gamma_u = 1 \forall u$) we would have, from (22), $e_{3,N}(\mathbf{z}) \to 0$ as $N \to \infty$, which in turn would imply (since $g \in H_3$) that $Q_{3,N}g \to I_3g$ (or $\mathbb{E}[(Q_{3,N}g - I_3g)^2] \to 0$ in the Sobolev case), contradicting the last part of the theorem.

Thus to prove the theorem we must prove the existence of a finite sequence of three-dimensional lattice rules which are very bad as 3-dimensional rules, yet for which all of the 1-dimensional and 2-dimensional projections are good in the sense of (24). This is our next task.

5 Proof of Theorem 4.1

In the proof we make use of the following well known property of lattice rules with a prime number of points. **Lemma 5.1** Let N be prime and $\mathbf{z} \in \mathbb{Z}^d$. If $a \not\equiv 0 \pmod{N}$ then

$$Q_{d,N}(a\mathbf{z}) = Q_{d,N}(\mathbf{z})$$

Proof: By definition,

$$Q_{d,N}(a\mathbf{z})f = \frac{1}{N}\sum_{j=0}^{N-1} f\left(\left\{\frac{ja\mathbf{z}}{N}\right\}\right).$$

Because N is prime and $a \not\equiv 0 \pmod{N}$ we have

$${ja: j = 0, \dots, N-1} = {j: j = 0, \dots, N-1} \pmod{N},$$

thus

$$Q_{d,N}(a\mathbf{z})f = \frac{1}{N}\sum_{j=0}^{N-1} f\left(\left\{\frac{j\mathbf{z}}{N}\right\}\right) = Q_{d,N}(\mathbf{z})f,$$

completing the proof.

It follows from this lemma that without loss of generality the first component of the generating vector can be chosen to be 1: provided $z_1 \not\equiv 0$ (mod N), we can replace the generating vector \mathbf{z} by $z_1^{-1}\mathbf{z}$, where z_1^{-1} denotes the unique integer in $\{1, \ldots, N-1\}$ that satisfies

$$z_1^{-1}z_1 \equiv 1 \pmod{N}.$$

We prove Theorem 4.1 by way of a construction and a series of lemmas. For the construction, we assume $N \geq 3$ and take the 3-dimensional lattice vector \mathbf{z} to be of the form

$$(z_1, z_2, z_3) = (1, v, w),$$

with $v \in \{1, 2, ..., N - 1\}$, and

$$w \equiv v + 1 \pmod{N}$$

(Later we shall show that v = N - 1 can be excluded, but it is convenient to allow this value of v in the following technical arguments.)

Thus our 3-dimensional lattice rule is

$$Q_{3,N}f = \frac{1}{N} \sum_{j=0}^{N-1} f\left(\frac{j}{N}, \left\{\frac{jv}{N}\right\}, \left\{\frac{j(v+1)}{N}\right\}\right)$$
$$= \frac{1}{N} \sum_{j=0}^{N-1} f(t_1^{(j)}, t_2^{(j)}, t_3^{(j)}), \qquad (25)$$

with

$$t_1^{(j)} = \frac{j}{N}, \qquad t_2^{(j)} = \left\{\frac{jv}{N}\right\}, \qquad t_3^{(j)} = \left\{t_1^{(j)} + t_2^{(j)}\right\}, \qquad j = 0, \dots, N-1.$$
(26)

We first observe that this is a very bad 3-dimensional rule. This is so because, for arbitrary N and arbitrary v, all the points $\mathbf{t}^{(j)} = \left(t_1^{(j)}, t_2^{(j)}, t_3^{(j)}\right)$ lie on two planes: since $t_1^{(j)} + t_2^{(j)} \in [0, 2)$, from the last equation in (26) we must have either $t_3^{(j)} = t_1^{(j)} + t_2^{(j)}$ or $t_3^{(j)} = t_1^{(j)} + t_2^{(j)} - 1$. In other words, all N points $\mathbf{t}^{(j)}$ lie on one or other of the planes in \mathbb{R}^3 defined by

$$x_1 + x_2 - x_3 = 0, \qquad x_1 + x_2 - x_3 = 1.$$

Now consider the function

$$g(x_1, x_2, x_3) := (x_1 + x_2 - x_3)^2 (x_1 + x_2 - x_3 - 1)^2$$
$$\times \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3) . \tag{27}$$

It is easy to see that g has a continuous periodic extension to \mathbb{R}^3 , and that it belongs to the Korobov space H_3 . It is also clear (since $g(\mathbf{x}) \ge 0 \forall \mathbf{x} \in [0, 1]^3$) that $I_3g > 0$; yet (since g vanishes on both of the planes that contain all the points $\mathbf{t}^{(j)}$) we have $Q_{3,N}(1, v, v + 1)g = 0$. Thus the existence of $g \in H_3$ for which $Q_3(\mathbf{z})g \not\rightarrow I_3g$, as needed in the last part of the theorem, has been proved for every $v \in \{1, \ldots, N-1\}$.

To show that (20) holds for some $v \in \{1, ..., N-1\}$, we make use of (23), which expresses the worst-case error in terms of the *u*-discrepancies of the projections of the lattice rule. It proves convenient to replace the 2-dimensional discrepancies in this expression by the 2-dimensional worst-case errors for the **un**weighted case, which we do by using the three identities typified by (from (18))

$$e_{2,N}(z_1, z_2)^2 = D_{1,N}(z_1)^2 + D_{1,N}(z_2)^2 + D_{2,N}(z_1, z_2)^2.$$

In this way (23) is replaced by

$$\begin{split} e_{3,N}^{\Gamma}(z_1, z_2, z_3)^2 &= (\Gamma_{\{1\}} - \Gamma_{\{1,2\}} - \Gamma_{\{1,3\}}) D_{1,N}(z_1)^2 \\ &+ (\Gamma_{\{2\}} - \Gamma_{\{1,2\}} - \Gamma_{\{2,3\}}) D_{1,N}(z_2)^2 \\ &+ (\Gamma_{\{3\}} - \Gamma_{\{1,3\}} - \Gamma_{\{2,3\}}) D_{1,N}(z_3)^2 \\ &+ \Gamma_{\{1,2\}} e_{2,N}(z_1, z_2)^2 + \Gamma_{\{2,3\}} e_{2,N}(z_2, z_3)^2 + \Gamma_{\{1,3\}} e_{2,N}(z_1, z_3)^2. \end{split}$$

The three 1-dimensional projections of the rule (25) are

$$\frac{1}{N}\sum_{j=0}^{N-1} f\left(\frac{j}{N}\right),\tag{28}$$

$$\frac{1}{N}\sum_{j=0}^{N-1} f\left(\left\{\frac{jv}{N}\right\}\right),\tag{29}$$

$$\frac{1}{N}\sum_{j=0}^{N-1} f\left(\left\{\frac{j(v+1)}{N}\right\}\right).$$
(30)

The discrepancy corresponding to the first 1-dimensional projection, given by (28), is from (15) and (14),

$$D_{1,N}(1) = \left[\frac{1}{N}\sum_{j=0}^{N-1} B_2\left(\frac{j}{N}\right)\right]^{1/2} = \left[\frac{1}{N}\sum_{j=0}^{N-1}\sum_{h\neq 0}\frac{e^{2\pi i h j/N}}{2\pi^2 h^2}\right]^{1/2}$$
$$= \left[\sum_{\substack{h\neq 0\\h\equiv 0(\text{mod }N)}}\frac{1}{2\pi^2 h^2}\right]^{1/2} = \left(\frac{B_2(0)}{N^2}\right)^{1/2} = \frac{1}{\sqrt{6}N}.$$
(31)

The second 1-dimensional projection (29) is (by Lemma 5.1) the same as the first, and so has the same discrepancy. So too has the third projection (30), unless v = N - 1 in which case the discrepancy is

$$D_{1,N}(0) = \left[\frac{1}{N}\sum_{j=0}^{N-1} B_2(0)\right]^{1/2} = \frac{1}{\sqrt{6}}.$$
(32)

Now we turn to the 2-dimensional projections. The three 2-dimensional projections of (25) are

$$\frac{1}{N} \sum_{j=0}^{N-1} f\left(\frac{j}{N}, \left\{\frac{jv}{N}\right\}\right),$$

$$\frac{1}{N} \sum_{j=0}^{N-1} f\left(\frac{j}{N}, \left\{\frac{j(v+1)}{N}\right\}\right),$$

$$\frac{1}{N} \sum_{j=0}^{N-1} f\left(\left\{\frac{jv}{N}\right\}, \left\{\frac{j(v+1)}{N}\right\}\right),$$

and the three corresponding 2-dimensional worst-case errors in the unweighted case are $e_{2,N}(1, v)$, $e_{2,N}(1, v+1)$ and $e_{2,N}(v, v+1)$. Denoting the corresponding root-mean-square averages of the unweighted worst case errors over all values of $v \in \{1, \ldots, N-1\}$ by $M_{2,N}^{xy}, M_{2,N}^{xz}$ and $M_{2,N}^{yz}$, we prove the following lemma:

Lemma 5.2 Let N be prime. Then

$$\max(M_{2,N}^{xy}, M_{2,N}^{xz}, M_{2,N}^{yz}) < \frac{\sqrt{2}}{\sqrt{N}}.$$

 $\mathbf{Proof} \ \mathbf{Since}$

$$(M_{2,N}^{xy})^2 = \frac{1}{N-1} \sum_{v=1}^{N-1} e_{2,N}(1,v)^2,$$

we already know from (19) that

$$M_{2,N}^{xy} \le \frac{7}{6\sqrt{N}} < \frac{\sqrt{2}}{\sqrt{N}}.$$

For the second mean we have

$$(M_{2,N}^{xz})^{2} = \frac{1}{N-1} \sum_{v=1}^{N-1} e_{2,N} (1, v+1)^{2}$$
$$= \frac{1}{N-1} \left[\sum_{w=1}^{N-1} e_{2,N} (1, w)^{2} + e_{2,N} (1, 0)^{2} - e_{2,N} (1, 1)^{2} \right]$$
$$\leq (M_{2,N}^{xy})^{2} + \frac{1}{N-1} e_{2,N} (1, 0)^{2}.$$

From (16) we have

$$e_{2,N}(1,0)^2 = -1 + \frac{1}{N} \sum_{j=0}^{N-1} \left(1 + B_2(0) \right) \left(1 + B_2\left(\frac{j}{N}\right) \right)$$
$$= -1 + \frac{7}{6} + \frac{7}{6N} \sum_{j=0}^{N-1} B_2\left(\frac{j}{N}\right)$$
$$= \frac{1}{6} + \frac{7}{36N^2},$$

where we used $B_2(0) = 1/6$, and used (31) for the sum $\sum_{j=0}^{N-1} B_2(j/N) = 1/(6N)$. Using $N \ge 2$ and the bound for $M_{2,N}^{xy}$ we obtain easily

$$\left(M_{2,N}^{xz}\right)^2 \le \frac{49}{36N} + \frac{1}{4N} + \frac{7}{6 \times 36N} < \frac{2}{N}.$$

Finally, for the third mean we have,

$$(M_{2,N}^{yz})^2 = \frac{1}{N-1} \sum_{v=1}^{N-1} e_{2,N}(v,v+1)^2$$

and using Lemma 5.1

$$(M_{2,N}^{yz})^2 = \frac{1}{N-1} \sum_{v=1}^{N-1} e_{2,N} (1, v^{-1}(v+1))^2$$
$$= \frac{1}{N-1} \sum_{v=1}^{N-1} e_{2,N} (1, v^{-1}+1)^2$$
$$= \frac{1}{N-1} \sum_{w=1}^{N-1} e_{2,N} (1, w+1)^2$$
$$= (M_{2,N}^{xz})^2 < \frac{2}{N},$$

where we used the fact that with N prime

$$\{v^{-1}: 1 \le v \le N - 1\} = \{w: 1 \le w \le N - 1\}.$$

This completes the proof of the lemma.

The next step is to show that there is at least one value of $v \in \{1, 2, ..., N-1\}$ for which all three 2-dimensional worst-case errors are small simultaneously. To that end we use the following elementary lemma. **Lemma 5.3** Let $\{a_1, \ldots, a_n\} \subseteq \mathbb{R}$ be a sequence of non-negative numbers, and let \bar{a} be their mean. Then for all $\lambda > 1$

$$|\{i \in \{1,\ldots,n\}: a_i \le \lambda \overline{a}\}| \ge \left(1 - \frac{1}{\lambda}\right) n.$$

Proof. Suppose the contrary. Then for some $\lambda > 1$ we have

$$|\{i \in \{1, \dots, n\} : a_i \le \lambda \bar{a}\}| < \left(1 - \frac{1}{\lambda}\right)n,$$

or equivalently

$$|\{i \in \{1, \dots, n\} : a_i > \lambda \overline{a}\}| \ge n - \left(1 - \frac{1}{\lambda}\right)n = \frac{n}{\lambda},$$

and hence

$$\bar{a} = \frac{1}{n} \sum_{i=1}^{n} a_i \ge \frac{1}{n} \sum_{i:a_i > \lambda \bar{a}} a_i > \frac{1}{n} \frac{n}{\lambda} \lambda \bar{a} = \bar{a},$$

which is a contradiction.

Corollary 5.4 Let N be prime and $\lambda > 3$. Then

$$\left| \left\{ v \in \{1, \dots, N-1\} : \max\left(e_{2,N}(1,v)^2, e_{2,N}(1,v+1)^2, e_{2,N}(v,v+1)^2\right) \le \frac{2\lambda}{N} \right\} \right|$$
$$\ge \left(1 - \frac{3}{\lambda}\right) (N-1).$$

Proof. It follows from the last lemma that

$$|\{v \in \{1, \dots, N-1\} : e_{2,N}(1,v)^2 \le \lambda (M_{2,N}^{xy})^2\}| \ge \left(1 - \frac{1}{\lambda}\right) (N-1) ,$$

and hence from Lemma 5.2

$$\left| \left\{ v \in \{1, \dots, N-1\} : e_{2,N}(1,v)^2 \le \frac{2\lambda}{N} \right\} \right| \ge \left(1 - \frac{1}{\lambda}\right) (N-1) ,$$

Similarly,

$$\left| \left\{ v \in \{1, \dots, N-1\} : e_{2,N}(1, v+1)^2 \le \frac{2\lambda}{N} \right\} \right| \ge \left(1 - \frac{1}{\lambda}\right) (N-1) ,$$

and

$$\left|\left\{v \in \{1, \dots, N-1\} : e_{2,N}(v, v+1)^2 \le \frac{2\lambda}{N}\right\}\right| \ge \left(1 - \frac{1}{\lambda}\right)(N-1).$$

It follows that the cardinality of the set of the $v \in \{1, ..., N-1\}$ such that

$$e_{2,N}(1,v)^2 \le \frac{2\lambda}{N}$$
 and $e_{2,N}(1,v+1)^2 \le \frac{2\lambda}{N}$

is at least $\left(1-\frac{1}{\lambda}\right)(N-1) + \left(1-\frac{1}{\lambda}\right)(N-1) - (N-1) = 1 - \frac{2}{\lambda}(N-1)$, since $\lambda > 2$. In turn it follows that the cardinality of the set of the $v \in \{1, \ldots, N-1\}$ such that all three of the squared 2-dimensional worst-case errors have the bound $2\lambda/N$ is at least

$$\left(1-\frac{2}{\lambda}\right)(N-1) + \left(1-\frac{1}{\lambda}\right)(N-1) - (N-1) = \left(1-\frac{3}{\lambda}\right)(N-1)$$

since $\lambda > 3$, and the corollary is proved.

Now return to the proof of Theorem 4.1. Since $\mathbf{z} = (1, v, v+1)$, it follows from the last corollary, provided $(1 - 3/\lambda)(N - 1) \ge 1$, that there exists $\mathbf{z} \in \{1, \ldots, N\}^3$ satisfying (20). The condition is satisfied if, for example, $\lambda = 6$ and $N \ge 3$.

We have so far allowed $v \in \{1, \ldots, N-1\}$ in the averaging arguments, therefore leaving open the possibility that $z_3 = N$. To show that v = N - 1cannot occur except possibly for a finite number of values of N, first we assume $\Gamma_{\{3\}} \neq 0$. Suppose that v = N - 1 occurs for some unbounded sequence of primes N. Then for such values of N we would have (see (32))

$$D_{1,N}(z_3) = D_{1,N}(N) = D_{1,N}(0) = 1/\sqrt{6},$$

and hence from (23) $e_{3,N}(\mathbf{z}) \neq 0$ as $N \to \infty$, contradicting the bound (20) in the theorem. If $\Gamma_{\{3\}} = 0$ we carry out the construction again but with the value of $\Gamma_{\{3\}}$ changed to 1, since the \mathbf{z} so constructed will still have the required properties even for the problem with $\Gamma_{\{3\}} = 0$. The resulting vcannot equal N-1 for an unbounded sequence of primes N. Thus the result in Theorem 1 holds for all sufficiently large primes N. It therefore holds for all primes N, possibly with a larger value of the constant c_{Γ} . This completes the proof of Theorem 4.1.

6 Proof of Theorem 4.2

To prove Theorem 4.2, we may use exactly the same construction for the vector \mathbf{z} as in the previous section, thus

$$Q_{3,N}(\mathbf{z}, \mathbf{\Delta})f = \frac{1}{N} \sum_{j=0}^{N-1} f\left(\left\{\frac{j}{N} + \Delta_1\right\}, \left\{\frac{jv}{N} + \Delta_2\right\}, \left\{\frac{j(v+1)}{N} + \Delta_3\right\}\right),$$

where v is found exactly as in Section 5. The bound (21) then follows from (20) using the equality of $e_{2,N}^{\Gamma,\text{sh}}$ with $e_{2,N}^{\Gamma}$ established in Section 3. For the function g we may replace (27) by the simpler expression

$$g(x_1, x_2, x_3) := (x_1 + x_2 - x_3)^2 (x_1 + x_2 - x_3 - 1)^2,$$

since the Sobolev space setting does not impose periodic boundary conditions. The shifted lattice rule $Q_{3,N}(\mathbf{z}, \boldsymbol{\Delta})$ from (13) is then an equal weight sum of values ranging from 0 (achieved with $\boldsymbol{\Delta} = \mathbf{0}$) to 4 (which is the maximum value of g on the closed unit cube, almost achieved when $j = 0, \Delta_1 = \Delta_2 = 1-, \Delta_3 = 0$). When N is large the distribution of the values of $Q_{3,N}(\mathbf{z}, \boldsymbol{\Delta})g$ between these extremes becomes essentially independent of N, from which it is clear that $\mathbb{E}[(Q_{3,N}(\mathbf{z}, \boldsymbol{\Delta})g - I_3g)^2] \neq 0$.

7 Discussion

Now we return to the case of general dimensionality d, and suppose that f (in the Sobolev case) is a fixed function of d variables for which all mixed first derivatives are square integrable, and also (in the Korobov case) that f is periodic with respect to each of the d variables. The integral $I_d f$ is to be integrated by a rank-1 lattice rule $Q_{d,N}f$ constructed by the CBC algorithm. The question is: how should the weights Γ be chosen?

If the weights are chosen to be of the classical product form (5) then $f \in H_d^{\Gamma}$, and it follows from [7] that

$$|I_d f - Q_{d,N} f| \le \frac{C_{\Gamma,\Delta}}{N^{1-\delta}} ||f||_{H^{\Gamma}_d} , \qquad (33)$$

in the Korobov case, while in the Sobolev case the same result is obtained for the root-mean-square error averaged over shifts. Thus we have a guaranteed optimal rate of convergence no matter how the product weights are chosen. The choice of weights still matters, since it affects both the constant in (33) and the size of the norm of f. One might reasonably try, in a similar manner to [9, 3], to choose product weights that minimise the error bound (33).

In marked contrast, if the weights Γ are chosen to be of the order-2 form (i.e. $\Gamma_u = 0$ for $|u| \ge 3$) then because the CBC algorithm at each step tries to minimise the worst-case error, which now has the form (see (10))

$$e_{d,N}^{\Gamma}(\mathbf{z})^2 = \sum_{0 < |u| \le 2} \Gamma_u D_{|u|,N}(\mathbf{z}_u),$$

the algorithm completely ignores the quality of 3-dimensional and higher dimensional projections. This observation tells us that there is no guarantee of convergence: for example, Theorem 4.1 indicates for the Korobov case that convergence could fail even for a function of just the first three variables, e.g.

$$f(x_1,\ldots,x_d) = g(x_1,x_2,x_3),$$

with g given by (27).

Similar concerns apply with equal force to finite-order weights of higher order q, unless f is known to be exactly expressible as a sum of functions of at most q variables at a time.

It seems a reasonable conclusion that for most applications the use of finite-order weights in the CBC algorithm for constructing lattice integration rules lacks theoretical justification, and can even be dangerous.

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