Fast CBC construction of randomly shifted lattice rules achieving $\mathcal{O}(n^{-1+\delta})$ convergence for unbounded integrands over $\mathbb{R}^s$ in weighted spaces with POD weights

James A. Nichols and Frances Y. Kuo

School of Mathematics and Statistics, University of NSW, Sydney NSW 2052, Australia

Abstract

This paper provides the theoretical foundation for the component-by-component (CBC) construction of randomly shifted lattice rules that are tailored to integrals over $\mathbb{R}^s$ arising from practical applications. For an integral of the form $\int_{\mathbb{R}^s} f(\boldsymbol{y}) \prod_{j=1}^s \phi(y_j)\,\mathrm{d}\boldsymbol{y}$ with a univariate probability density ϕ, our general strategy is to first map the integral into the unit cube $[0,1]^s$ using the inverse of the cumulative distribution function of ϕ, and then apply quasi-Monte Carlo (QMC) methods. However, the transformed integrand in the unit cube rarely falls within the standard QMC setting of Sobolev spaces of functions with mixed first derivatives. Therefore, a non-standard function space setting for integrands over $\mathbb{R}^s$, previously considered by Kuo, Sloan, Wasilkowski and Waterhouse (J. Complexity, 2010), is required for the analysis. Motivated by the needs of three applications, the present paper extends the theory of the aforementioned paper in several nontrivial directions, including a new error analysis for the CBC construction of lattice rules with general non-product weights, the introduction of an unanchored variant for the setting, the use of coordinate-dependent weight functions in the norm, and the strategy for fast CBC construction with POD ("product and order dependent") weights.

Keywords: Unbounded integrands, POD weights, Randomly shifted lattice rules, Quasi-Monte Carlo methods, General weights

1. Introduction

High dimensional integrals arise from many practical applications in the form of multivariate expected values. Often these practical integrals are formulated over the Euclidean space $\mathbb{R}^s$, and frequently the quantity of interest is integrated

Email address: james.nichols@student.unsw.edu.au, f.kuo@unsw.edu.au (James A. Nichols and Frances Y. Kuo)

with respect to the multivariate Gaussian density with a specified mean and covariance structure. Examples include, but by no means are limited to, integrals arising from option pricing problems in finance e.g. [7, 1, 33, 20, 23, 24], maximum likelihood problems in statistics e.g. [10, 11, 47, 26, 39], and porous media flow problems in computational physics e.g. [9, 35, 36, 46, 21, 22]. In these practical applications, the number of variables s can be as high as hundreds or thousands, or even infinite. The aim of this paper is to provide the theoretical foundation for the *fast component-by-component* (CBC) *construction of randomly shifted lattice rules* that are tailored to these practical integrals. In Section 2 we will discuss three motivating applications, and outline how the theory of this paper can be applied.

Quasi-Monte Carlo (QMC) methods are equal-weight quadrature rules for approximating integrals over the unit cube $[0,1]^s$. In recent years, great advances have been made in the analysis of QMC methods in very high dimensions. The "standard" setting assumes that the integrand belongs to some "weighted" Sobolev space containing functions whose mixed first derivatives are square integrable e.g. [41, 42, 16, 19]. By now it is known that constructive QMC methods, most notably the family of randomly shifted lattice rules, can achieve nearly the optimal rate of convergence $\mathcal{O}(n^{-1})$ in the standard setting, where n is the number of QMC sample points, and where the implied constant can be independent of the dimension s under appropriate conditions on the "weight parameters", see e.g. [40, 25, 12, 37, 38, 8, 18]. Moreover, *digital nets* achieving the higher order $\mathcal{O}(n^{-r})$ for $r > 1$ are also known, see e.g. [13, 14, 6, 17, 5].

A necessary first step in applying QMC methods to a practical integral formulated over $\mathbb{R}^s$ is to transform the integral into the unit cube $[0,1]^s$. After some appropriate manipulations (some problem-specific strategies will be outlined in Section 2), a practical integral over $\mathbb{R}^s$ can be rewritten in the form

$$\int_{\mathbb{R}^s} f(\boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\,\mathrm{d}\boldsymbol{y} \;=\; \int_{[0,1]^s} f(\Phi^{-1}(\boldsymbol{u}))\,\mathrm{d}\boldsymbol{u}, \tag{1}$$

where ϕ is a univariate probability density function on $\mathbb{R}$, while Φ^{-1} denotes the inverse of the corresponding cumulative distribution function, which, when applied to vectors is done component-wise. A QMC method with points $\boldsymbol{t}^{(1)}, \ldots, \boldsymbol{t}^{(n)} \in [0,1]^s$ then approximates the last integral in (1) by

$$\frac{1}{n} \sum_{k=1}^{n} f(\Phi^{-1}(\boldsymbol{t}^{(k)})). \tag{2}$$

However, the transformation in (1) often results in an integrand $f(\Phi^{-1}(\cdot))$ that is either unbounded at the boundary of the unit cube, or has unbounded derivatives near the boundary. In those cases, the standard QMC theory cannot be applied.

An "anchored" function space over $\mathbb{R}^s$ was considered in [31], see also [44, 45, 32]. It was shown that randomly shifted lattice rules can be obtained using a CBC construction to achieve close to the optimal convergence rate in this

non-standard setting. To understand the setting it is instructive to examine the details of the norm defined by

$$\|f\|^2 = \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^{|\mathfrak{u}|}} \left(\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} f(\boldsymbol{y}_{\mathfrak{u}}; \mathbf{0})\right)^2 \prod_{j\in\mathfrak{u}} \psi^2(y_j)\,\mathrm{d}\boldsymbol{y}_{\mathfrak{u}}. \tag{3}$$

Here $\{1:s\}$ is a shorthand for the set of indices $\{1,2,\ldots,s\}$, $\frac{\partial^{|\mathfrak{u}|} f}{\partial \boldsymbol{y}_{\mathfrak{u}}}$ denotes the mixed first partial derivatives of f with respect to the "active" variables $\boldsymbol{y}_{\mathfrak{u}} := (y_j)_{j\in\mathfrak{u}}$, and $(\boldsymbol{y}_{\mathfrak{u}}; \mathbf{0})$ is the vector obtained from $\boldsymbol{y}$ by "anchoring" those "inactive" variables $\boldsymbol{y}_{-\mathfrak{u}} := (y_j)_{j\notin\mathfrak{u}}$ to the value 0. This function space setting has three key ingredients:

- The *univariate probability density* $\phi : \mathbb{R} \to \mathbb{R}\setminus\mathbb{R}^-$ in (1) controls the mapping from $\mathbb{R}^s$ to the unit cube $[0,1]^s$. Although ϕ does not affect the norm (3), it determines the transformed integrand $f(\Phi^{-1}(\cdot))$ over the unit cube.

- The positive and continuous *weight function* $\psi : \mathbb{R} \to \mathbb{R}^+$ in the norm (3) controls the boundary behavior of the functions f that are included in the space. If $\psi(y_j)$ decays very quickly to 0 for large $|y_j|$ then the space can contain functions with very fast diverging mixed derivatives.

- The collection of *weight parameters* $\gamma_{\mathfrak{u}}$ associated with subsets $\mathfrak{u} \subset \mathbb{N}$ with finite cardinality $|\mathfrak{u}| < \infty$ controls the relative importance of various groups of variables: a small $\gamma_{\mathfrak{u}}$ quantifies weak dependence of the function f on the group of variables $\boldsymbol{y}_{\mathfrak{u}}$.

We remark that here we take the point of view that ϕ is something we can choose rather than being a fixed entity. Although it may seem natural to consider ϕ to be fixed, particularly when considering integrals that are expectations with respect to that distribution, in practice the integral is easy to modify. Thus it is up to the practitioner to *choose an appropriate density* ϕ (for example, simply divide and multiply the given integral by the product of ϕ). This is particularly important as in practical applications the associated integral will often *not* be in the form (1). Having chosen ϕ, it is then important to *choose a weight function* ψ to make the corresponding norm (3) finite and small. It is also crucial to *choose the weight parameters* $\gamma_{\mathfrak{u}}$ to ensure that the QMC quadrature errors are small, and preferably bounded independently of the dimension s. Hence, it is through a careful choice of ϕ, ψ, and $\gamma_{\mathfrak{u}}$ that the theory of randomly shifted lattice rules can be applied rigorously to practical integrals formulated over $\mathbb{R}^s$. In Section 2 we will explain that the choice of ϕ played the crucial role for maximum likelihood problems [26, 31, 39], whereas a non-trivial choice of ψ was the key step for PDE problems with lognormal random coefficients [22]. The choice of weight parameters $\gamma_{\mathfrak{u}}$ was vital in both applications.

This paper provides a number of important extensions to the theory in [31], all motivated by the needs of practical applications. Firstly, we removed the assumption that the weight parameters $\gamma_{\mathfrak{u}}$ take the product form $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$.

Such a generalization was considered in [19, 42] for the standard setting over the unit cube. This generalization was prompted by the analysis from the recent application of QMC to PDE applications [28, 29], where it was found that the overall error bound is minimized when the weight parameters take the form of "POD weights", which is short for "product and order dependent weights":

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j, \tag{4}$$

that is, the weight parameters are determined by the choice of two sequences $\Gamma_0 = \Gamma_1 = 1, \Gamma_2, \ldots$ and $\gamma_1, \gamma_2, \ldots$. This generalization means that the theoretical basis for the CBC construction of randomly shifted lattice rules in this non-standard setting needs to be proved anew, and this non-trivial result is the main theorem of this paper.

As highlighted in [15] for the standard setting, the CBC construction with general non-product weights in the anchored setting has an issue with the computational cost due to the need to work with some "auxiliary weights". The same issue holds for the non-standard setting considered here. Our second major advance in this paper is to introduce an "unanchored" version of the function space over $\mathbb{R}^s$. The norm (3) is changed to

$$\|f\|^2 = \sum_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^{|\mathfrak{u}|}} \left(\int_{\mathbb{R}^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} f(\boldsymbol{y}_{\mathfrak{u}}; \boldsymbol{y}_{\text{-}\mathfrak{u}}) \prod_{j \notin \mathfrak{u}} \phi(y_j) \, \mathrm{d}\boldsymbol{y}_{\text{-}\mathfrak{u}} \right)^2 \prod_{j \in \mathfrak{u}} \psi^2(y_j) \, \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}, \tag{5}$$

where, instead of anchoring the inactive variables $\boldsymbol{y}_{\text{-}\mathfrak{u}}$ to 0, they are simply integrated out with respect to the density ϕ. We provide the complete theory for the CBC construction in this unanchored variant, and discuss the computational strategies for implementing fast CBC construction with POD weights.

Similarly to the standard setting over $[0,1]^s$, the unanchored variant of our function space has a natural connection with the "ANOVA decomposition" of functions over $\mathbb{R}^s$, while the anchored variant connects with the anchored decomposition, see [30]. Thus the theory of this paper can be applied to the smooth ANOVA terms of the integrand arising from option pricing problems, see [24] and below.

In addition to the two major extensions, we also make other generalizations. We allow the weight parameters $\gamma_{\mathfrak{u}}$ to depend on the dimension s: later we write, more explicitly, $\gamma_{s,\mathfrak{u}}$. This is natural for the maximum likelihood problems [39] since all model parameters depend on the dimension s. This is also useful from the point of view of linking the theory between anchored and unanchored settings. We allow the weight function ψ to be coordinate-dependent, that is, we have a weight function ψ_j for each coordinate. This turns out to be a crucial step in modeling the PDE applications in [22]. In our analysis we also allow the integration domain to be more general, to cater for other potential future applications.

The outline of this paper is as follows. In Section 2 we discuss three practical applications that motivate the theoretical developments of this paper, and outline how the theory can be applied in each case. In Section 3 we discuss the function space settings of this paper, briefly surveying the literature of reproducing kernel Hilbert spaces, and introduce the expression for the shift-averaged worst-case errors for randomly shifted lattice rules in this setting. In Subsection 3.3 we review known results in the anchored setting, and then in Subsection 3.4 we derive various results in the new unanchored setting. In Section 4 we present the CBC algorithm for constructing a good generating vector of randomly shifted lattice rules, and then prove the main convergence results of the shift-averaged worst-case error for both the anchored and unanchored spaces with general non-product weights. In Section 5 we discuss issues in implementation of the CBC algorithm, and present ways of circumventing some numerical problems we encountered along the way. Finally in Section 6 we present numerical results from our implementation of the CBC algorithm for the unanchored setting with POD weights.

2. Motivating applications

Integrals over $\mathbb{R}^s$ often arise from practical applications in the form of multivariate expected values

$$\mathbb{E}_\rho[q] \;=\; \int_{\mathbb{R}^s} q(\boldsymbol{y})\,\rho(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}, \tag{6}$$

where q is some quantity of interest which depends on a vector $\boldsymbol{y} = (y_1, \ldots, y_s)$ of parameters or variables in s dimensions, and ρ is some multivariate probability density function, not necessarily a product of univariate functions, describing the distribution of $\boldsymbol{y}$. Below we discuss three motivating applications.

2.1. Application to PDE problems with lognormal random coefficients

Our first example, taken from [22], concerns fluid flow through a porous medium, typically modelled using Darcy's Law, with random coefficients. The governing PDE is

$$-\nabla\cdot(a(\boldsymbol{x},\omega)\,\nabla u(\boldsymbol{x},\omega)) = \chi(\boldsymbol{x}) \quad \text{for almost all } \omega\in\Omega, \text{ and } \boldsymbol{x}\in D\subset\mathbb{R}^d, \tag{7}$$

with $d\in\{1,2,3\}$, subject to homogeneous Dirichlet boundary conditions. The coefficient $a(\boldsymbol{x},\omega)$ is assumed to be a log-normal random field representing the permeability of a porous material over the spatial domain D, and Ω is the probability space. That is, $a(\boldsymbol{x},\omega) := \exp(Z(\boldsymbol{x},\omega))$ where $Z(\boldsymbol{x},\omega)$ is a zero-mean homogenous Gaussian field characterized by an isotropic covariance kernel.

The goal is to compute the expectations $\mathbb{E}[G(u)]$ of linear functionals $G(\cdot)$ of the solution u over Ω. Using the Karhunen-Loève expansion we can parameterize the probability space Ω, and we can write

$$Z(\boldsymbol{x},\omega) \;=\; \sum_{j=1}^{\infty} \sqrt{\mu_j}\,\xi_j(\boldsymbol{x})\,y_j(\omega)\,,$$

where μ_j are real, positive and non-increasing in j, the ξ_j are orthonormal in $L_2(D)$, and $(y_j(\omega))_{j\geq 1}$ is a sequence of i.i.d. standard normal $\mathcal{N}(0,1)$ random variables. The field can then be approximated by truncating the expansion at s terms. The expectation $\mathbb{E}[G(u)]$, using the truncated expansion, can therefore be expressed in the form of the integral in (1), with $f(\boldsymbol{y}) = G(u(\cdot, \boldsymbol{y}))$ and with ϕ being the standard normal probability density. The PDE can be solved for each $\boldsymbol{y}$ using finite element methods.

One crucial step in the analysis of [22] is to choose suitable weight functions ψ_j so that the function $f(\boldsymbol{y}) = G(u(\cdot, \boldsymbol{y}))$ has a finite and indeed small norm (5), so that the CBC error bound of this paper can be applied. Another crucial step in [22] is to choose the weight parameters $\gamma_{\mathfrak{u}}$ to minimize the overall error bound while ensuring that the bound holds independently of s. This yields weights of the POD form, and the fast CBC implementation of this paper can be used. In summary, this paper provides the theoretical and practical foundations for [22].

2.2. Application to option pricing problems

Following the Black-Scholes model, integrals arising from option pricing problems take the general form of (6), with

$$q(\boldsymbol{y}) = \max(\mu(\boldsymbol{y}), 0) \quad \text{and} \quad \rho(\boldsymbol{y}) = \frac{\exp(-\frac{1}{2}\boldsymbol{y}^{\mathsf{T}}\Sigma^{-1}\boldsymbol{y})}{\sqrt{(2\pi)^s \det(\Sigma)}},$$

where the variables $\boldsymbol{y} = (y_1, \ldots, y_s)^{\mathsf{T}}$ correspond to a discretization of the underlying Brownian motion over a time interval $[0, T]$, and the covariance matrix has entries $\Sigma_{ij} = (T/s)\min(i, j)$. For example, in the case of an "arithmetic average Asian call option", the payoff function q depends on the smooth function $\mu(\boldsymbol{y}) = (1/s)\sum_{j=1}^{s} S_{t_j}(\boldsymbol{y}) - K$ which is the difference between the average of the asset prices S_{t_j} at the discrete times and the strike price K.

The widely accepted strategy to rewrite these option pricing integrals in the form (1) is to take a factorization $\Sigma = AA^{\mathsf{T}}$ and apply a change of variables $\boldsymbol{y} = A\boldsymbol{y}'$. This yields $f(\boldsymbol{y}') = q(A\boldsymbol{y}')$, with ϕ being the standard normal density. The choice of factorization therefore determines the function f. For example, A can be obtained through Cholesky factorization ("standard construction"), through "Brownian bridge construction" (see [7]), or eigenvalue decomposition (sometimes called the "principal component construction", see [1]).

The success of QMC for option pricing cannot be explained by most existing theory due to the "kink" in the integrand. However, for some factorizations it is shown in [24] that all "ANOVA terms" of f are smooth, with the exception of the highest order term. It remains to show that these smooth ANOVA terms belong to the unanchored setting of this paper so that the present theory can be applied; this is work in progress.

2.3. Application to maximum likelihood problems

Another source of inspiration towards the non-standard setting in this paper is a class of generalized response models in statistics, as examined in [26, 31, 39].

A specific example of the time series Poisson likelihood model considered in these papers involves an integral of the form (6), with

$$q(\boldsymbol{y}) = \prod_{j=1}^{s} \frac{\exp(\tau_j(\beta + y_j) - e^{\beta+y_j})}{\tau_j!} \quad \text{and} \quad \rho(\boldsymbol{y}) = \frac{\exp(-\frac{1}{2}\boldsymbol{y}^{\mathrm{T}}\Sigma^{-1}\boldsymbol{y})}{\sqrt{(2\pi)^s \det(\Sigma)}}.$$

Here $\beta \in \mathbb{R}$ is a model parameter, $\tau_1, \ldots, \tau_s \in \{0, 1, \ldots\}$ are the count data, and Σ is a Toeplitz covariance matrix with $\Sigma_{ij} = \sigma^2\kappa^{|i-j|}/(1-\kappa^2)$, where σ^2 is the variance and $\kappa \in (-1, 1)$ is the autoregression coefficient.

An obvious way to rewrite this integral in the form (1) is to factorize Σ as discussed above for the option pricing applications, but this would yield a very spiky function f. Instead, the strategy developed in [26] recenters and rescales the exponent of the integrand $q(\boldsymbol{y})\rho(\boldsymbol{y}) = \exp(F(\boldsymbol{y}))$ as follows: (i) find the unique stationary point $\boldsymbol{y}^*$ satisfying $\nabla F(\boldsymbol{y}^*) = 0$, (ii) determine the matrix $\Sigma^* = (-\nabla^2 F(\boldsymbol{y}^*))^{-1}$ which describes the convexity of F around the stationary point, (iii) factorise $\Sigma^* = A^*A^{*\mathrm{T}}$, (iv) apply a change of variables $\boldsymbol{y} = A^*\boldsymbol{y}' + \boldsymbol{y}^*$, (v) multiply and divide the resulting integrand by a product of some univariate densities ϕ. These steps then yield an integral of the form (1) with $f(\boldsymbol{y}') = c\exp(F(A^*\boldsymbol{y}' + \boldsymbol{y}^*))/(\prod_{j=1}^{s}\phi(y_j'))$ for some scaling constant $c > 0$. Note that the choice of A^* and ϕ determines f.

Using the results from this current paper and following the strategy for choosing weight parameters in [28, 29], the recent paper [39] provides careful estimates of the norm of the resulting integrand f corresponding to three different choices of density ϕ, with the weight function taken as $\psi \equiv 1$, and gives the formula for the weight parameters $\gamma_{\mathfrak{u}}$ that minimize the overall error bound.

3. Function space setting

3.1. General framework of reproducing kernel Hilbert spaces

First we review the general framework of the function space setting from [32]. Suppose that our domain is $D := \overline{(a, b)}$, allowing unbounded intervals such as $\mathbb{R}$. Let ϕ be a univariate probability density function on D, that is, $\phi(y) \geq 0$ for all $y \in D$ and $\int_a^b \phi(y)\,\mathrm{d}y = 1$. We define the cumulative distribution function $\Phi : D \to [0, 1]$ as

$$\Phi(y) := \int_a^y \phi(t)\,\mathrm{d}t,$$

and denote its inverse by $\Phi^{-1} : [0, 1] \to D$. For $s \geq 1$, we are interested in the integral of a function $f : D^s \to \mathbb{R}$ with respect to the product probability density, that is

$$I_{s,\phi}(f) := \int_{D^s} f(\boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\,\mathrm{d}\boldsymbol{y}.$$

We assume that the integrand f belongs to a weighted reproducing kernel Hilbert space (RKHS) $\mathcal{F}$ of real valued functions on D^s. A reproducing kernel

is a function $K_{\mathcal{F}} : D^s \times D^s \to \mathbb{R}$ that satisfies $K_{\mathcal{F}}(\cdot, \boldsymbol{y}) \in \mathcal{F}$ for all $\boldsymbol{y} \in D^s$, $K_{\mathcal{F}}(\boldsymbol{x}, \boldsymbol{y}) = K_{\mathcal{F}}(\boldsymbol{y}, \boldsymbol{x})$ for all $\boldsymbol{x}, \boldsymbol{y} \in D^s$, and the *reproducing property*

$$\langle f, K_{\mathcal{F}}(\cdot, \boldsymbol{y})\rangle_{\mathcal{F}} = f(\boldsymbol{y}) \quad \text{for all } f \in \mathcal{F} \text{ and } \boldsymbol{y} \in D^s. \tag{8}$$

For an in-depth analysis of RKHS, see [2].

To ensure the embedding of $\mathcal{F}$ in $L_{2,\phi}(D^s)$, which is required in our later analysis, and to ensure that $I_{s,\phi}(f)$ is well-defined, we assume that

$$\int_{D^s} K_{\mathcal{F}}(\boldsymbol{y}, \boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y} < \infty. \tag{9}$$

Using (8), we can now express the integral $I_{s,\phi}(f)$ for any $f \in \mathcal{F}$ in terms of the reproducing kernel

$$I_{s,\phi}(f) \;=\; \int_{D^s} \langle f, K_{\mathcal{F}}(\cdot, \boldsymbol{y})\rangle_{\mathcal{F}} \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y} \;=\; \langle f, h\rangle_{\mathcal{F}},$$

where

$$h(\boldsymbol{x}) := \int_{D^s} K_{\mathcal{F}}(\boldsymbol{x}, \boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y}$$

is the *representer of integration* in $\mathcal{F}$. Assumption (9) implies that $I_{s,\phi}(f)$ and h are well defined, in fact we see that

$$\begin{aligned}
|I_{s,\phi}(f)| \;&\le\; \int_{D^s} \|f\|_{\mathcal{F}}\, \|K_{\mathcal{F}}(\cdot, \boldsymbol{y})\|_{\mathcal{F}} \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y} \\
&=\; \|f\|_{\mathcal{F}} \int_{D^s} [K_{\mathcal{F}}(\boldsymbol{y}, \boldsymbol{y})]^{1/2} \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y} \\
&\le\; \|f\|_{\mathcal{F}} \left(\int_{D^s} K_{\mathcal{F}}(\boldsymbol{y}, \boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\, \mathrm{d}\boldsymbol{y} \right)^{1/2} \;<\; \infty\,.
\end{aligned}$$

where the second inequality is obtained using Cauchy-Schwarz inequality The *initial error* of integration,

$$e_{s,0}(\mathcal{F}) := \sup_{\|f\|_{\mathcal{F}} \le 1} |I_{s,\phi}(f)| \;=\; \langle h, h\rangle_{\mathcal{F}}^{1/2},$$

is then guaranteed to be finite as $h \in \mathcal{F}$, hence we have

$$[e_{s,0}(\mathcal{F})]^2 = \|h\|_{\mathcal{F}}^2 = \int_{D^s} \int_{D^s} K_{\mathcal{F}}(\boldsymbol{x}, \boldsymbol{y}) \prod_{j=1}^{s} (\phi(x_j)\, \phi(y_j))\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y} < \infty. \tag{10}$$

To be able to apply QMC methods, we must map the integrand from the Hilbert space $\mathcal{F}$ of functions on D^s to a Hilbert space $\mathcal{G}$ of functions on $[0,1]^s$, where we use the isometry

$$f \in \mathcal{F} \iff g = f(\Phi^{-1}(\cdot)) \in \mathcal{G}, \quad \text{with} \quad \|f\|_{\mathcal{F}} = \|g\|_{\mathcal{G}}.$$

Note that we implicitly used the short-hand component wise notation, $\Phi^{-1}(\boldsymbol{u}) = (\Phi^{-1}(u_1), \dots, \Phi^{-1}(u_s))$. It is important to note that the integral remains the same under this isometry,

$$I_{s,\phi}(f) = I_s(g) := \int_{[0,1]^s} g(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}.$$

The space $\mathcal{G}$ is also a RKHS, where the kernel is

$$K_{\mathcal{G}}(\boldsymbol{u}, \boldsymbol{v}) = K_{\mathcal{F}}(\Phi^{-1}(\boldsymbol{u}), \Phi^{-1}(\boldsymbol{v})), \quad \boldsymbol{u},\, \boldsymbol{v} \in [0,1]^s. \tag{11}$$

Later we will need the associated shift-invariant kernel

$$\begin{aligned} K_{\mathcal{G}}^{\mathrm{sh}}(\boldsymbol{u}, \boldsymbol{v}) &:= \int_{[0,1]^s} K_{\mathcal{G}}(\{\boldsymbol{u} + \boldsymbol{\Delta}\}, \{\boldsymbol{v} + \boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta} \\ &= \int_{[0,1]^s} K_{\mathcal{F}}(\Phi^{-1}(\{\boldsymbol{u} + \boldsymbol{\Delta}\}), \Phi^{-1}(\{\boldsymbol{v} + \boldsymbol{\Delta}\}))\,\mathrm{d}\boldsymbol{\Delta}, \end{aligned} \tag{12}$$

where $\{x\} = x - \lfloor x \rfloor$ represents taking the fractional part of a number, and should be applied component-wise to a vector. Note that the shift-invariant kernel is actually a function of one variable, as it depends only on the difference of the two points $\boldsymbol{u}$ and $\boldsymbol{v}$. With a slight abuse of notation we write

$$K_{\mathcal{G}}^{\mathrm{sh}}(\boldsymbol{u}, \boldsymbol{v}) = K_{\mathcal{G}}^{\mathrm{sh}}(\{\boldsymbol{u} - \boldsymbol{v}\}, \boldsymbol{0}) = K_{\mathcal{G}}^{\mathrm{sh}}(\{\boldsymbol{u} - \boldsymbol{v}\}).$$

The initial error of integration in $\mathcal{G}$ is the same as in the original space $\mathcal{F}$,

$$e_{s,0}(\mathcal{G}) \;=\; \sup_{\|g\|_{\mathcal{G}} \le 1} |I_s(g)| \;=\; \sup_{\|f\|_{\mathcal{F}} \le 1} |I_{s,\phi}(f)| \;=\; e_{s,0}(\mathcal{F}).$$

We approximate the integral $I_s(g)$ by a QMC rule

$$Q_{s,n}(g) \;=\; \frac{1}{n} \sum_{k=1}^{n} g(\boldsymbol{t}^{(k)}),$$

with points $\boldsymbol{t}^{(1)}, \dots, \boldsymbol{t}^{(n)} \in [0,1]^s$, and it is in this space $\mathcal{G}$ that we can study the *worst-case error*, defined as

$$e^{\mathrm{wor}}(Q_{s,n}; \mathcal{G}) \;=\; \sup_{\|g\|_{\mathcal{G}} \le 1} |I_s(g) - Q_{s,n}(g)|.$$

Then it is straightforward to relate this to the original integration problem for $f \in \mathcal{F}$,

$$\begin{aligned} |I_{s,\phi}(f) - Q_{s,n}(f \circ \Phi^{-1})| \;&=\; |I_s(g) - Q_{s,n}(g)| \\ &\le\; e^{\mathrm{wor}}(Q_{s,n}; \mathcal{G})\, \|g\|_{\mathcal{G}} \;=\; e^{\mathrm{wor}}(Q_{s,n}; \mathcal{G})\, \|f\|_{\mathcal{F}}. \end{aligned} \tag{13}$$

The last expression illustrates the fact that while we study the worst-case error in $\mathcal{G}$, for which we have explicit expressions, we can keep the analysis of the norm of f in the original space $\mathcal{F}$, which is more convenient.

3.2. Randomly shifted lattice rules

We focus on randomly shifted lattice rules for numerical integration in the space $\mathcal{G}$. Let

$$\mathcal{Z}_n := \{z \in \mathbb{Z} : 1 \le z \le n \text{ and } \gcd(z,n) = 1\}$$

denote the set of positive integers between 1 and n that are relatively prime to n. Given a *generating vector* $\boldsymbol{z} \in \mathcal{Z}_n^s$ and a *shift* $\boldsymbol{\Delta} \in [0,1]^s$ (usually taken to be a vector of i.i.d. uniformly distributed numbers), the points $\{\boldsymbol{t}^{(k)}\}_{k=1}^n$ of the shifted (rank-1) lattice rule are given by

$$\boldsymbol{t}^{(k)} = \left\{ \frac{k\boldsymbol{z}}{n} + \boldsymbol{\Delta} \right\}, \qquad k = 1, \ldots, n,$$

where the braces indicate taking the fractional parts of a vector as in (12). As we consider *randomly* shifted lattice rules, we are interested in the *shift-averaged worst-case error*, which now only depends on $\boldsymbol{z}$ and is well-known (see e.g., [40]) to reduce to

$$\begin{aligned}[e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2 &:= \int_{[0,1]^s} [e^{\mathrm{wor}}(Q_{s,n}; \mathcal{G})]^2 \,\mathrm{d}\boldsymbol{\Delta} \\ &= -\int_{[0,1]^s} \int_{[0,1]^s} K_{\mathcal{G}}(\boldsymbol{u}, \boldsymbol{v}) \,\mathrm{d}\boldsymbol{u} \,\mathrm{d}\boldsymbol{v} + \frac{1}{n} \sum_{k=1}^n K^{\mathrm{sh}}_{\mathcal{G}} \left(\left\{ \frac{k\boldsymbol{z}}{n} \right\} \right). \end{aligned} \tag{14}$$

3.3. Anchored spaces

Here we recap the *weighted anchored spaces* as studied in [32, 31], but with some new developments. Given an anchor $c \in D$, a set of *weight parameters* $\gamma_{s,\mathrm{u}} > 0$ (or "weights" for short) and a set of *weight functions* $\psi_j : D \to \mathbb{R}$, the space $\mathcal{F}$ is the Hilbert space of functions from D^s to $\mathbb{R}$ with the inner-product

$$\langle f, g \rangle_{\mathcal{F}} = \sum_{\mathrm{u} \subseteq \{1:s\}} \frac{1}{\gamma_{s,\mathrm{u}}} \int_{D^{|\mathrm{u}|}} \frac{\partial^{|\mathrm{u}|} f}{\partial \boldsymbol{y}_{\mathrm{u}}}(\boldsymbol{y}_{\mathrm{u}}; \boldsymbol{c}) \, \frac{\partial^{|\mathrm{u}|} g}{\partial \boldsymbol{y}_{\mathrm{u}}}(\boldsymbol{y}_{\mathrm{u}}; \boldsymbol{c}) \prod_{j \in \mathrm{u}} \psi_j^2(y_j) \,\mathrm{d}\boldsymbol{y}_{\mathrm{u}}, \tag{15}$$

where the notation is as in (3), but with a general domain D and a general anchor value c instead of 0. We take $\gamma_{s,\emptyset} = 1$. As usual the corresponding norm is $\|f\|_{\mathcal{F}} = \langle f, f \rangle_{\mathcal{F}}^{1/2}$. The generalisations from (3) to (15) include the allowance for general (non-product) weights $\gamma_{s,\mathrm{u}}$, which may depend on the dimension s, as well as for coordinate-dependent weight functions ψ_j. The role of the weight parameters $\gamma_{s,\mathrm{u}}$ and weight functions ψ_j have been explained in the introduction.

The reproducing kernel corresponding to the inner product (15) is given by

$$K_{\mathcal{F}}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\mathrm{u} \subseteq \{1:s\}} \gamma_{s,\mathrm{u}} \prod_{j \in \mathrm{u}} \eta_j(x_j, y_j), \tag{16}$$

where for $x,\, y \in D$,

$$\eta_j(x,y) = \begin{cases} \displaystyle\int_c^{\min(x,y)} \frac{1}{\psi_j^2(t)}\,\mathrm{d}t & \text{if } x,\, y > c, \\ \displaystyle\int_{\max(x,y)}^{c} \frac{1}{\psi_j^2(t)}\,\mathrm{d}t & \text{if } x,\, y < c, \\ 0 & \text{otherwise.} \end{cases}$$

For this to be well-defined we must assume that for all j, ψ_j satisfies

$$\int_x^y \frac{1}{\psi_j^2(t)}\,\mathrm{d}t < \infty \quad \text{for all finite } x \text{ and } y. \tag{17}$$

The change from product weights to general weights means that the reproducing kernel is no longer of a product form, and this affects the error analysis of lattice rules significantly. The additional dependence of the weights $\gamma_{s,\mathfrak{u}}$ on the dimension s and the coordinate-dependent weight functions ψ_j can be considered to be trivial generalizations from the error analysis point of view, but they affect the construction cost for lattice rules.

We examine the two quantities (9) and (10). Substituting (16) into (10), we find that

$$\int_{D^s}\int_{D^s} K_{\mathcal{F}}(\boldsymbol{x},\boldsymbol{y}) \prod_{j=1}^{s} (\phi(x_j)\phi(y_j))\;\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}} C_{0,j}, \tag{18}$$

where we define

$$\begin{aligned} C_{0,j} &:= \int_a^b \int_a^b \eta_j(x_j,y_j)\,\phi(x_j)\,\phi(y_j)\,\mathrm{d}x_j\mathrm{d}y_j \\ &= \int_a^c \frac{\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t + \int_c^b \frac{(1-\Phi(t))^2}{\psi_j^2(t)}\,\mathrm{d}t, \end{aligned} \tag{19}$$

with the last equality demonstrated in [31]. Similarly, we see that (9) reduces to

$$\int_{D^s} K_{\mathcal{F}}(\boldsymbol{y},\boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j)\,\mathrm{d}\boldsymbol{y} = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}} C_{1,j}, \tag{20}$$

where we define

$$\begin{aligned} C_{1,j} &:= \int_a^b \eta_j(y_j,y_j)\,\phi(y_j)\,\mathrm{d}y_j \\ &= \int_a^c \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t + \int_c^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t, \end{aligned} \tag{21}$$

with the last equality again shown in [31]. Evidently, to satisfy (9) we require that $C_{1,j} < \infty$ for all j. As this implies the boundedness of (10), we furthermore have $C_{0,j} < \infty$ for all j.

Now we turn to the corresponding function space $\mathcal{G}$. The kernel $K_{\mathcal{G}}(\boldsymbol{u}, \boldsymbol{v})$ can be calculated as in (11), while the associated shift-invariant kernel is

$$K_{\mathcal{G}}^{\mathrm{sh}}(\{\boldsymbol{u}-\boldsymbol{v}\}) = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}} \theta_j(\{u_j - v_j\}), \tag{22}$$

where

$$\begin{aligned}\theta_j(u) &:= \int_0^1 \eta_j(\Phi^{-1}(\{u+\Delta\}), \Phi^{-1}(\Delta))\,\mathrm{d}\Delta \\ &= \int_{\Phi^{-1}(u)}^{c} \frac{\Phi(t)-u}{\psi_j^2(t)}\,\mathrm{d}t + \int_{\Phi^{-1}(1-u)}^{c} \frac{\Phi(t)-1+u}{\psi_j^2(t)}\,\mathrm{d}t, \qquad u\in[0,1],\end{aligned} \tag{23}$$

which was derived in [32]. It is important to note that

$$C_{0,j} = \int_0^1 \theta_j(u)\,\mathrm{d}u \qquad \text{and} \qquad C_{1,j} = \theta_j(0),$$

which holds regardless of the precise formula for η_j, hence this applies in the unanchored space, examined in the next subsection.

Now we are in a position to express the shift-averaged worst-case error for lattice rules in the anchored space. Substituting (18) and (22) into (14), we obtain the expression

$$[e_{s,n}^{\mathrm{sh}}(\boldsymbol{z})]^2 = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \left(-\prod_{j\in\mathfrak{u}} C_{0,j} + \frac{1}{n}\sum_{k=1}^{n}\prod_{j\in\mathfrak{u}} \theta_j\left(\left\{\frac{kz_j}{n}\right\}\right)\right). \tag{24}$$

3.4. Unanchored spaces

Here we introduce the *weighted unanchored spaces*. We commence by deriving the reproducing kernel in one dimension, and then proceed to higher dimensions where we also derive results for the shift-averaged worst-case errors for lattice rules.

Note here that the anchored and unanchored spaces have kernels that share a similar structure, with the principal difference being the definition of η_j. The formulas or definitions in (16)–(24) are hence also valid in the unanchored spaces, however we must calculate new formulas for the quantities $C_{0,j}$, $C_{1,j}$ and θ_j that depend on η_j.

Lemma 1 (Unanchored space – reproducing kernel) *We take $\mathcal{F}$ to be the space of absolutely continuous functions from D to $\mathbb{R}$ whose first derivatives are square-integrable when multiplied by the square of a weight function $\psi_j : D \to \mathbb{R}^+$ satisfying* (17)*. We define the inner product of $f, g \in \mathcal{F}$ as*

$$\langle f, g\rangle_{\mathcal{F}} := \left(\int_a^b f(y)\,\phi(y)\,\mathrm{d}y\right)\left(\int_a^b g(y)\,\phi(y)\,\mathrm{d}y\right) + \frac{1}{\gamma}\int_a^b f'(y)\,g'(y)\,\psi_j^2(y)\,\mathrm{d}y,$$

with $\gamma > 0$. Then the reproducing kernel in $\mathcal{F}$ is given by $K_{\mathcal{F}}(x,y) = 1 + \gamma\eta_j(x,y)$, where

$$\eta_j(x,y) \;=\; \int_a^{\min(x,y)} \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t + \int_{\max(x,y)}^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t. \tag{25}$$

Proof. Since this reproducing kernel does not appear to exist in the literature, rather than simply verifying the reproducing property, we provide a derivation.

Suppose that $K_{\mathcal{F}}(x,y) = 1 + \gamma\eta_j(x,y)$, with

$$\eta_j(x,y) \;=\; \begin{cases} L_x(y) & \text{for } y \le x, \\ R_x(y) & \text{for } y \ge x, \end{cases}$$

where, for every $x \in D$, $L_x(y)$ and $R_x(y)$ are absolutely continuous functions in y whose first derivatives are square-integrable when multiplied by $\psi_j^2(y)$, and they satisfy $L_x(x) = R_x(x)$. For any $f \in \mathcal{F}$, the reproducing property (8) yields

$$\begin{aligned} f(x) \;=\; &\left(\int_a^b f(y)\,\phi(y)\,\mathrm{d}y\right)\left(1 + \gamma\left[\int_a^x L_x(y)\,\phi(y)\,\mathrm{d}y + \int_x^b R_x(y)\,\phi(y)\,\mathrm{d}y\right]\right) \\ &+ \int_a^x f'(y)\,L_x'(y)\,\psi_j^2(y)\,\mathrm{d}y \;+\; \int_x^b f'(y)\,R_x'(y)\,\psi_j^2(y)\,\mathrm{d}y. \end{aligned}$$

Since this must hold for all $\gamma > 0$, we conclude that

$$\begin{cases} \displaystyle\int_a^x L_x(y)\,\phi(y)\,\mathrm{d}y + \int_x^b R_x(y)\,\phi(y)\,\mathrm{d}y \;=\; 0, \\ \displaystyle\int_a^x f'(y)\,L_x'(y)\,\psi_j^2(y)\,\mathrm{d}y + \int_x^b f'(y)\,R_x'(y)\,\psi_j^2(y)\,\mathrm{d}y = f(x) - \int_a^b f(y)\,\phi(y)\,\mathrm{d}y. \end{cases} \tag{26}$$

As an initial guess, we assume that

$$L_x'(y) \;=\; \frac{\ell_x(y)}{\psi_j^2(y)} \qquad \text{and} \qquad R_x'(y) \;=\; \frac{r_x(y)}{\psi_j^2(y)}$$

for suitably defined functions $\ell_x(y)$ and $r_x(y)$ to be specified below. Defining $M(x) := L_x(x) = R_x(x)$, we can write

$$L_x(y) \;=\; M(x) - \int_y^x \frac{\ell_x(t)}{\psi_j^2(t)}\,\mathrm{d}t \qquad \text{and} \qquad R_x(y) \;=\; M(x) + \int_x^y \frac{r_x(t)}{\psi_j^2(t)}\,\mathrm{d}t. \tag{27}$$

Then the two required properties in (26) simplify to (assuming that all integrals are finite and therefore interchanging the order of integration is allowed)

$$\begin{cases} \displaystyle\int_a^x \frac{\Phi(t)\,\ell_x(t)}{\psi_j^2(t)}\,\mathrm{d}t \;-\; \int_x^b \frac{(1-\Phi(t))\,r_x(t)}{\psi_j^2(t)}\,\mathrm{d}t \;=\; M(x) \\ \displaystyle\int_a^x f'(y)\,\ell_x(y)\,\mathrm{d}y \;+\; \int_x^b f'(y)\,r_x(y)\,\mathrm{d}y \;=\; f(x) - \int_a^b f(y)\,\phi(y)\,\mathrm{d}y. \end{cases} \tag{28}$$

If we take

$$\ell_x(y) \,=\, \Phi(y) \qquad \text{and} \qquad r_x(y) \,=\, \Phi(y) - 1, \tag{29}$$

then it can be verified using integration by parts that the second equation in (28) holds. Substituting (29) into the first equation in (28) determines $M(x)$.

Finally we express $\eta_j(x,y)$ as in (25). Consider first the case $y \le x$. Then from (27), (28), and (29) we have for $y \le x$ that

$$\begin{aligned}\eta_j(x,y) \,=\, L_x(y) \,&=\, \int_a^x \frac{\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t \,+\, \int_x^b \frac{(1-\Phi(t))^2}{\psi_j^2(t)}\,\mathrm{d}t \,-\, \int_y^x \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t \\ &=\, \int_a^y \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t \,+\, \int_x^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t \,-\, \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t.\end{aligned}$$

We easily obtain a similar expression for $x \le y$, hence obtaining (25). □

We can now generalize the unanchored setting to s dimensions. The unanchored inner product is

$$\begin{aligned}\langle f, g\rangle_{\mathcal{F}} \,:=\, \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{s,\mathfrak{u}}} \int_{D^{|\mathfrak{u}|}} \Bigg(\int_{D^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} f}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}; \boldsymbol{y}_{\text{-}\mathfrak{u}}) \prod_{j\notin\mathfrak{u}} \phi(y_j)\,\mathrm{d}\boldsymbol{y}_{\text{-}\mathfrak{u}} \Bigg) \\ \times \Bigg(\int_{D^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} g}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}_{\mathfrak{u}}; \boldsymbol{y}_{\text{-}\mathfrak{u}}) \prod_{j\notin\mathfrak{u}} \phi(y_j)\,\mathrm{d}\boldsymbol{y}_{\text{-}\mathfrak{u}} \Bigg) \prod_{j\in\mathfrak{u}} \psi_j^2(y_j)\,\mathrm{d}\boldsymbol{y}_{\mathfrak{u}},\end{aligned} \tag{30}$$

where the notation is as in (5). The reproducing kernel takes the same form as (16), but now with the function η_j defined by (25). As before we require the two conditions (18) and (20), but now with different constants $C_{0,j}$ and $C_{1,j}$.

Lemma 2 (Unanchored space – constants) *For the function η_j given by (25), the quantities $C_{0,j}$ and $C_{1,j}$ defined in (19) and (21), respectively, are*

$$C_{0,j} \,=\, 0 \qquad \text{and} \qquad C_{1,j} \,=\, \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t.$$

Proof. Substituting (25) into (19), we have that

$$\begin{aligned} C_{0,j} \,&=\, \int_a^b \int_a^b \int_a^{\min(x,y)} \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t\,\phi(x)\phi(y)\,\mathrm{d}x\,\mathrm{d}y \\ &\quad + \int_a^b \int_a^b \int_{\max(x,y)}^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t\,\phi(x)\phi(y)\,\mathrm{d}x\,\mathrm{d}y - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t \\ &= \int_a^b \frac{\Phi(t)}{\psi_j^2(t)} \int_t^b \int_t^b \phi(x)\phi(y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t \\ &\quad + \int_a^b \frac{1-\Phi(t)}{\psi_j^2(t)} \int_a^t \int_a^t \phi(x)\phi(y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t \\ &= \int_a^b \frac{\Phi(t)(1-\Phi(t))^2}{\psi_j^2(t)}\,\mathrm{d}t + \int_a^b \frac{(1-\Phi(t))\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t, \end{aligned}$$

which equals 0. Similarly, substituting (25) into (21), we obtain

$$
\begin{aligned}
&C_{1,j} \\
&= \int_a^b \int_a^x \frac{\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t\, \phi(x) \,\mathrm{d}x + \int_a^b \int_x^b \frac{1-\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t\, \phi(x) \,\mathrm{d}x - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)} \,\mathrm{d}t \\
&= \int_a^b \frac{\Phi(t)}{\psi_j^2(t)} \int_t^b \phi(x) \,\mathrm{d}x \,\mathrm{d}t + \int_a^b \frac{1-\Phi(t)}{\psi_j^2(t)} \int_a^t \phi(x) \,\mathrm{d}x \,\mathrm{d}t - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)} \,\mathrm{d}t,
\end{aligned}
$$

which simplifies to the required expression. □

Now we consider the space $\mathcal{G}$ of functions on the unit cube. The kernel $K_{\mathcal{G}}(\boldsymbol{u}, \boldsymbol{v})$ is given by (11), and the associated shift invariant kernel $K_{\mathcal{G}}^{\mathrm{sh}}(\{\boldsymbol{u}-\boldsymbol{v}\})$ is of the same form as (22), but the function θ_j takes a different form.

Lemma 3 (Unanchored space – shift-invariant kernel) *For the function η_j given by* (25)*, the function θ_j defined in* (23) *is*

$$
\theta_j(u) = \int_{\Phi^{-1}(u)}^b \frac{\Phi(t)-u}{\psi_j^2(t)} \,\mathrm{d}t + \int_{\Phi^{-1}(1-u)}^b \frac{\Phi(t)-1+u}{\psi_j^2(t)} \,\mathrm{d}t - \int_a^b \frac{\Phi^2(t)}{\psi_j^2(t)} \,\mathrm{d}t. \quad (31)
$$

Alternatively, given any arbitrary point $c \in D$, we can express θ_j as

$$
\begin{aligned}
\theta_j(u) = &\int_{\Phi^{-1}(u)}^c \frac{\Phi(t)-u}{\psi_j^2(t)} \,\mathrm{d}t + \int_{\Phi^{-1}(1-u)}^c \frac{\Phi(t)-1+u}{\psi_j^2(t)} \,\mathrm{d}t \\
&- \int_a^c \frac{\Phi^2(t)}{\psi_j^2(t)} \,\mathrm{d}t - \int_c^b \frac{(1-\Phi(t))^2}{\psi_j^2(t)} \,\mathrm{d}t. \quad (32)
\end{aligned}
$$

Note that the alternative expression (32) enables us to directly compare the unanchored space to the anchored space. If we use the superscripts 'anch' and 'unanch' to distinguish relevant quantities from the anchored and unanchored spaces, then

$$
\theta_j^{\mathrm{unanch}} = \theta_j^{\mathrm{anch}} - C_{0,j}^{\mathrm{anch}}. \quad (33)
$$

Proof. Substituting (25) into (23), we have

$$
\begin{aligned}
\theta_j(u) = &\int_0^1 \int_a^{\min(\Phi^{-1}(\{u+\Delta\}),\Phi^{-1}(\Delta))} \frac{\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta \\
&+ \int_0^1 \int_{\max(\Phi^{-1}(\{u+\Delta\}),\Phi^{-1}(\Delta))}^b \frac{1-\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta - \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)} \,\mathrm{d}t \\
= &\underbrace{\int_0^{1-u} \int_a^{\Phi^{-1}(\Delta)} \frac{\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta}_{A} + \int_{1-u}^1 \int_a^{\Phi^{-1}(u+\Delta-1)} \frac{\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta \\
&+ \int_0^{1-u} \int_{\Phi^{-1}(u+\Delta)}^b \frac{1-\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta + \int_{1-u}^1 \int_{\Phi^{-1}(\Delta)}^b \frac{1-\Phi(t)}{\psi_j^2(t)} \,\mathrm{d}t \,\mathrm{d}\Delta \\
&- \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)} \,\mathrm{d}t. \quad (34)
\end{aligned}
$$

For the expression labelled A, we substitute $w = \Phi^{-1}(\Delta)$ to obtain

$$A = \int_a^{\Phi^{-1}(1-u)} \int_a^w \frac{\Phi(t)}{\psi_j^2(t)}\,\mathrm{d}t\,\phi(w)\,\mathrm{d}w = \int_a^{\Phi^{-1}(1-u)} \frac{\Phi(t)}{\psi_j^2(t)} \int_t^{\Phi^{-1}(1-u)} \phi(w)\,\mathrm{d}w\,\mathrm{d}t$$
$$= \int_a^{\Phi^{-1}(1-u)} \frac{\Phi(t)}{\psi_j^2(t)}\,[(1-u)-\Phi(t)]\,\mathrm{d}t.$$

Applying a similar procedure to the rest of (34), we obtain

$$\begin{aligned}\theta_j(u) = &\int_a^{\Phi^{-1}(1-u)} \frac{\Phi(t)}{\psi_j^2(t)}\,[(1-u)-\Phi(t)]\,\mathrm{d}t + \int_a^{\Phi^{-1}(u)} \frac{\Phi(t)}{\psi_j^2(t)}\,[u-\Phi(t)]\,\mathrm{d}t\\ &+ \int_{\Phi^{-1}(u)}^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,[\Phi(t)-u]\,\mathrm{d}t + \int_{\Phi^{-1}(1-u)}^b \frac{1-\Phi(t)}{\psi_j^2(t)}\,[\Phi(t)-(1-u)]\,\mathrm{d}t\\ &- \int_a^b \frac{\Phi(t)(1-\Phi(t))}{\psi_j^2(t)}\,\mathrm{d}t,\end{aligned}$$

which simplifies to (31). Now, given some $c \in D$, we can rewrite (31) as

$$\begin{aligned}\theta_j(u) = &\int_{\Phi^{-1}(u)}^c \frac{\Phi(t)-u}{\psi_j^2(t)}\mathrm{d}t + \int_{\Phi^{-1}(1-u)}^c \frac{\Phi(t)-1+u}{\psi_j^2(t)}\mathrm{d}t\\ &+ \int_c^b \frac{\Phi(t)-u}{\psi_j^2(t)}\mathrm{d}t + \int_c^b \frac{\Phi(t)-1+u}{\psi_j^2(t)}\mathrm{d}t - \int_a^c \frac{\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t - \int_c^b \frac{\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t,\end{aligned}$$

which yields (32). □

Now we can express the shift-averaged worst-case error for lattice rules in the unanchored setting. It is also important to note that, as $C_{0,j} = 0$ in this space, we have $e_{s,0} = 1$. Substituting (18), (22), and $C_{0,j} = 0$ into (14), we obtain

$$[e_{s,n}^{\mathrm{sh}}(\boldsymbol{z})]^2 = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \frac{\gamma_{s,\mathfrak{u}}}{n} \sum_{k=1}^{n} \prod_{j \in \mathfrak{u}} \theta_j \left(\left\{ \frac{kz_j}{n} \right\} \right), \tag{35}$$

where θ_j is given by (31).

4. Main results

4.1. Reformulating the shift-averaged worst-case error for lattice rules

In Sections 3.3 and 3.4 we derived expressions for the shift-averaged worst-case error for lattice rules in the anchored and unanchored spaces. Here we reformulate the worst-case error in terms of the Fourier series coefficients of θ_j. We denote the Fourier coefficients by $\widehat{\theta}_j(h)$, where $h \in \mathbb{Z}$. We also write $\widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h}) = \prod_{j \in \mathfrak{v}} \widehat{\theta}_j(h_j)$ for $\boldsymbol{h} \in \mathbb{Z}^{|\mathfrak{v}|}$. For the anchored space it was shown in [31] that

$$\widehat{\theta}_j(h) = \frac{1}{\pi^2 h^2} \int_a^b \frac{1}{\psi_j^2(t)} \sin^2(\pi h \Phi(t))\,\mathrm{d}t \qquad \text{for} \quad h \neq 0. \tag{36}$$

We see from (33) that the function θ_j for the unanchored space only differs from the anchored case by a constant. Hence the formula (36) also applies in the unanchored space. Note from (36) that $\widehat{\theta}_j(h)$ for $h \neq 0$ are clearly all real and positive, and for both the anchored and unanchored spaces we have $C_{0,j} = \widehat{\theta}_j(0)$, while $C_{1,j} = \theta_j(0) = \sum_{h\in\mathbb{Z}} \widehat{\theta}_j(h)$.

In the following we use the notation $i \equiv_n j$ to mean $i \equiv j \pmod n$. First we consider the anchored case.

Lemma 4 *If we define a set of* auxiliary weights

$$\widetilde{\gamma}_{s,\mathfrak{v}} := \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}\setminus\mathfrak{v}} C_{0,j}, \qquad \mathfrak{v} \subseteq \{1:s\}, \tag{37}$$

then we can rewrite the shift-averaged worst-case error (24) *for the anchored space as*

$$[e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2 = \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}} \widetilde{\gamma}_{s,\mathfrak{v}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}}\equiv_n 0}} \widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h}), \tag{38}$$

where $\boldsymbol{z}_{\mathfrak{v}} \in \mathcal{Z}_n^{|\mathfrak{v}|}$ denotes the vector containing the components of the lattice generating vector $\boldsymbol{z} \in \mathcal{Z}_n^s$ whose indices are in $\mathfrak{v}$.

Proof. We rearrange the following sum over $\mathfrak{u}$ using the auxiliary weights such that the $h = 0$ term is removed from the Fourier representation:

$$\begin{aligned}
\sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}} \theta_j(x_j) &= \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \prod_{j\in\mathfrak{u}} \Big((\theta_j(x_j) - \widehat{\theta}_j(0)) + \widehat{\theta}_j(0)\Big) \\
&= \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \sum_{\mathfrak{v}\subseteq\mathfrak{u}} \Big(\prod_{j\in\mathfrak{u}\setminus\mathfrak{v}} \widehat{\theta}_j(0)\Big) \prod_{j\in\mathfrak{v}} \Big(\theta_j(x_j) - \widehat{\theta}_j(0)\Big) \\
&= \sum_{\mathfrak{v}\subseteq\{1:s\}} \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \Big(\prod_{j\in\mathfrak{u}\setminus\mathfrak{v}} C_{0,j}\Big) \prod_{j\in\mathfrak{v}} \Big(\theta_j(x_j) - \widehat{\theta}_j(0)\Big) \\
&= \sum_{\mathfrak{v}\subseteq\{1:s\}} \widetilde{\gamma}_{s,\mathfrak{v}} \prod_{j\in\mathfrak{v}} \Big(\theta_j(x_j) - \widehat{\theta}_j(0)\Big),
\end{aligned}$$

where $x_j = \{kz_j/n\}$. Thus (24) becomes

$$\begin{aligned}
[e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2 &= -\widetilde{\gamma}_{s,\emptyset} + \frac{1}{n}\sum_{k=1}^{n} \sum_{\mathfrak{v}\subseteq\{1:s\}} \widetilde{\gamma}_{s,\mathfrak{v}} \prod_{j\in\mathfrak{v}} \left[\theta_j\Big(\left\{\frac{kz_j}{n}\right\}\Big) - \widehat{\theta}_j(0)\right] \qquad (39) \\
&= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}} \frac{\widetilde{\gamma}_{s,\mathfrak{v}}}{n} \sum_{k=1}^{n} \prod_{j\in\mathfrak{v}} \sum_{h\in\mathbb{Z}\setminus\{0\}} \widehat{\theta}_j(h)\, e^{2\pi \mathrm{i} k h z_j/n} \\
&= \sum_{\emptyset\neq\mathfrak{v}\subseteq\{1:s\}} \frac{\widetilde{\gamma}_{s,\mathfrak{v}}}{n} \sum_{k=1}^{n} \sum_{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|}} \widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h})\, e^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}}/n}.
\end{aligned}$$

Applying the identity

$$\frac{1}{n}\sum_{k=1}^{n} e^{2\pi \mathrm{i} k \boldsymbol{h}\cdot \boldsymbol{z}_{\mathfrak{v}}/n} = \begin{cases} 1 & \text{if } \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}} \equiv_n 0, \\ 0 & \text{otherwise,} \end{cases}$$

we then obtain the formula (38). □

In the unanchored case, the use of the auxiliary weights $\widetilde{\gamma}_{s,\mathfrak{v}}$ is unnecessary due to $\widehat{\theta}_j(0) = C_{0,j} = 0$ and $\widetilde{\gamma}_{s,\mathfrak{v}} = \gamma_{s,\mathfrak{v}}$. Hence we have the following lemma.

Lemma 5 *The shift-averaged worst-case error* (35) *for the unanchored space can be written as*

$$[e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2 = \sum_{\emptyset\ne\mathfrak{u}\subseteq\{1:s\}} \gamma_{s,\mathfrak{u}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{u}}\equiv_n 0}} \widehat{\theta}_{\mathfrak{u}}(\boldsymbol{h}).$$

4.2. Error bound for the CBC construction

In the previous subsection we showed that the shift-averaged worst-case errors for the anchored and unanchored spaces can be written in the same form in terms of the Fourier coefficients of θ_j. In this subsection we provide the error analysis for randomly-shifted lattice rules constructed using a component-by-component algorithm. For each $d = 1, 2, \ldots, s$ and $\boldsymbol{z} \in \mathcal{Z}_n^d$, we consider the quantity

$$E^2_{d,s}(\boldsymbol{z}) := \sum_{\emptyset\ne\mathfrak{v}\subseteq\{1:d\}} \widetilde{\gamma}_{s,\mathfrak{v}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}}\equiv_n 0}} \widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h}), \tag{40}$$

noting that the weights $\widetilde{\gamma}_{s,\mathfrak{v}}$ depend on s and not on d. Evidently $E^2_{s,s}(\boldsymbol{z}) = [e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2$, but in general $E^2_{d,s}(\boldsymbol{z}) \ne [e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2$ for $d < s$. A notable exception occurs in the unanchored space: if the weights are independent of s, then $\widetilde{\gamma}_{s,\mathfrak{v}} = \gamma_{s,\mathfrak{v}} = \gamma_{\mathfrak{v}}$ and hence $E^2_{d,s}(\boldsymbol{z}) = [e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2$ for all $d \le s$.

Algorithm 6 (CBC Algorithm) *For any $n \ge 2$ and $s \ge 2$*

1. *Set $z_1 = 1$.*
2. *For each $d = 2, 3, \ldots, s$ with $z_1, \ldots, z_{d-1}$ fixed, choose $z_d \in \mathcal{Z}_n$ such that $E^2_{d,s}(z_1, \ldots, z_{d-1}, z_d)$ is minimised.*

Let $\zeta(x) := \sum_{h=1}^{\infty} h^{-x}$ for $x > 1$ denote the Riemann zeta function. Let $\varphi(n)$ denote Euler's totient function, the size of the set $\mathcal{Z}_n$.

Theorem 7 (CBC error bound) *Consider either the anchored or unanchored space. Let $r_2 > 1/2$ be such that for each $j \in \{1 : s\}$ we have some $C_{2,j} > 0$ and $r_{2,j} \ge r_2$ such that*

$$\widehat{\theta}_j(h) \le \frac{C_{2,j}}{|h|^{2r_{2,j}}} \quad \text{for all} \quad h \ne 0. \tag{41}$$

Then a generating vector $\boldsymbol{z}^* \in \mathcal{Z}_n^s$ can be constructed by Algorithm 6 so that for any $\lambda \in (1/(2r_2), 1]$ and for every $d \in \{1:s\}$ we have

$$E_{d,s}^2(z_1^*, \ldots, z_d^*) \le \left(\frac{1}{\varphi(n)} \sum_{\emptyset \ne \mathfrak{v} \subseteq \{1:d\}} \widetilde{\gamma}_{s,\mathfrak{v}}^{\lambda} \prod_{j \in \mathfrak{v}} \left(2C_{2,j}^{\lambda} \zeta(2r_{2,j}\lambda)\right) \right)^{1/\lambda}. \tag{42}$$

Proof. First we demonstrate the bound in (42) for $d = 1$. We have

$$\begin{aligned} E_{1,s}^2(1) &= \widetilde{\gamma}_{s,\{1\}} \sum_{\substack{h \in \mathbb{Z}\setminus\{0\} \\ h \equiv_n 0}} \widehat{\theta}_1(h) \le \widetilde{\gamma}_{s,\{1\}} \left(\sum_{\substack{h \in \mathbb{Z}\setminus\{0\} \\ h \equiv_n 0}} \frac{C_{2,1}^{\lambda}}{|h|^{2r_{2,1}\lambda}} \right)^{1/\lambda} \\ &= \widetilde{\gamma}_{s,\{1\}} \left(\frac{2C_{2,1}^{\lambda}\zeta(2r_{2,1}\lambda)}{n^{2r_{2,1}\lambda}} \right)^{1/\lambda} \le \widetilde{\gamma}_{s,\{1\}} \left(\frac{2C_{2,1}^{\lambda}\zeta(2r_{2,1}\lambda)}{\varphi(n)} \right)^{1/\lambda}, \end{aligned}$$

where we used (41) and Jensen's inequality $\sum_k a_k \le (\sum_k a_k^{\lambda})^{1/\lambda}$ for all nonnegative a_k and $\lambda \in (1/(2r_2), 1]$, as well as $2r_{2,1}\lambda \ge 2r_2\lambda > 1$ and $\varphi(n) < n$.

Suppose now that (42) holds for some $d < s$, and we proceed to prove that the choice of z_{d+1}^* obtained from Algorithm 6 satisfies the same error bound (42), but with d replaced by $d+1$. We split the expression in $d+1$ dimensions according to whether $d+1 \in \mathfrak{v}$ or not,

$$\begin{aligned} E_{d+1,s}^2(z_1, \ldots, z_d, z_{d+1}) &= \sum_{\emptyset \ne \mathfrak{v} \subseteq \{1:d+1\}} \widetilde{\gamma}_{s,\mathfrak{v}} \sum_{\substack{\boldsymbol{h} \in (\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}} \equiv_n 0}} \widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h}) \\ &= E_{d,s}^2(z_1, \ldots, z_d) + T_{d+1,s}(z_{d+1}), \end{aligned} \tag{43}$$

where

$$T_{d+1,s}(z_{d+1}) := \sum_{d+1 \in \mathfrak{v} \subseteq \{1:d+1\}} \widetilde{\gamma}_{s,\mathfrak{v}} \sum_{\substack{\boldsymbol{h} \in (\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}} \equiv_n 0}} \widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h}).$$

The choice of $z_{d+1}^* \in \mathcal{Z}_n$ that minimises $E_{d+1}^2(\boldsymbol{z}, z_{d+1})$ is also the choice that minimises the $T_{d+1,s}(z_{d+1})$ term, hence we have $T_{d+1,s}(z_{d+1}^*) \le T_{d+1,s}(z_{d+1})$ for all $z_{d+1} \in \mathcal{Z}_n$. It then also holds that $T_{d+1,s}^{\lambda}(z_{d+1}^*) \le T_{d+1,s}^{\lambda}(z_{d+1})$ for all $\lambda \in (1/(2r_2), 1]$, and thus as z_{d+1}^* minimises the $T_{d+1,s}^{\lambda}(z_{d+1})$ term, it also beats the average

$$T_{d+1,s}^{\lambda}(z_{d+1}^*) \le \frac{1}{\varphi(n)} \sum_{z_{d+1} \in \mathcal{Z}_n} T_{d+1,s}^{\lambda}(z_{d+1}).$$

We now apply Jensen's inequality to obtain

$$T_{d+1,s}^{\lambda}(z_{d+1}^*) \le \frac{1}{\varphi(n)} \sum_{z_{d+1} \in \mathcal{Z}_n} \sum_{d+1 \in \mathfrak{v} \subseteq \{1:d+1\}} \widetilde{\gamma}_{s,\mathfrak{v}}^{\lambda} \sum_{\substack{\boldsymbol{h} \in (\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|} \\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}} \equiv_n 0}} [\widehat{\theta}_{\mathfrak{v}}(\boldsymbol{h})]^{\lambda}.$$

Next we split the sum over $\boldsymbol{h}$ depending on whether or not h_{d+1} is a multiple of n, and use (41),

$$
\begin{aligned}
&T^{\lambda}_{d+1,s}(z^*_{d+1}) \\
&\le \sum_{d+1\in\mathfrak{v}\subseteq\{1:d+1\}} \widetilde{\gamma}^{\lambda}_{s,\mathfrak{v}} \Bigg(\sum_{\substack{h_{d+1}\in\mathbb{Z}\setminus\{0\}\\ h_{d+1}\equiv_n 0}} \frac{C^{\lambda}_{2,d+1}}{|h_{d+1}|^{2r_{2,d+1}\lambda}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\equiv_n 0}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C^{\lambda}_{2,j}}{|h_j|^{2r_{2,j}\lambda}} \\
&\quad + \frac{1}{\varphi(n)} \sum_{z_{d+1}\in\mathcal{Z}_n} \sum_{\substack{h_{d+1}\in\mathbb{Z}\setminus\{0\}\\ h_{d+1}\not\equiv_n 0}} \frac{C^{\lambda}_{2,d+1}}{|h_{d+1}|^{2r_{2,d+1}\lambda}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\equiv_n -h_{d+1}z_{d+1}}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C^{\lambda}_{2,j}}{|h_j|^{2r_{2,j}\lambda}} \Bigg).
\end{aligned} \tag{44}
$$

For the first term inside the brackets in (44), we have

$$
\sum_{\substack{h_{d+1}\in\mathbb{Z}\setminus\{0\}\\ h_{d+1}\equiv_n 0}} \frac{C^{\lambda}_{2,d+1}}{|h_{d+1}|^{2r_{2,d+1}\lambda}} = \frac{2C^{\lambda}_{2,d+1}\zeta(2r_{2,d+1}\lambda)}{n^{2r_{2,d+1}\lambda}},
$$

and we write

$$
B := \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\equiv_n 0}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C^{\lambda}_{2,j}}{|h_j|^{2r_{2,j}\lambda}}.
$$

The second term inside the brackets in (44) can be rewritten as

$$
\frac{1}{\varphi(n)} \sum_{c=1}^{n-1} \sum_{z_{d+1}\in\mathcal{Z}_n} \sum_{\substack{h_{d+1}\in\mathbb{Z}\setminus\{0\}\\ h_{d+1}\equiv_n -cz^{-1}_{d+1}}} \frac{C^{\lambda}_{2,d+1}}{|h_{d+1}|^{2r_{2,d+1}\lambda}} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\equiv_n c}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C^{\lambda}_{2,j}}{|h_j|^{2r_{2,j}\lambda}}. \tag{45}
$$

Now note that for any $c \in \{1,\dots,n-1\}$, we have equality of the two sets $\{cz^{-1}_{d+1} \pmod n : z_{d+1}\in\mathcal{Z}_n\} = \{cz \pmod n : z\in\mathcal{Z}_n\}$. Furthermore if we let

$p = \gcd(c,n)$, then $\gcd(c/p, n/p) = 1$ and we have

$$\begin{aligned}
&\sum_{z_{d+1}\in\mathcal{Z}_n} \sum_{\substack{h_{d+1}\in\mathbb{Z}\setminus\{0\}\\ h_{d+1}\equiv_n -cz_{d+1}^{-1}}} \frac{C_{2,d+1}^{\lambda}}{|h_{d+1}|^{2r_{2,d+1}\lambda}} = \sum_{z\in\mathcal{Z}_n}\sum_{m\in\mathbb{Z}} \frac{C_{2,d+1}^{\lambda}}{|mn-cz|^{2r_{2,d+1}\lambda}} \\
&= p^{-2r_{2,d+1}\lambda} \sum_{z\in\mathcal{Z}_n}\sum_{m\in\mathbb{Z}} \frac{C_{2,d+1}^{\lambda}}{|m(n/p)-(c/p)z|^{2r_{2,d+1}\lambda}} \\
&= p^{-2r_{2,d+1}\lambda} \sum_{z\in\mathcal{Z}_n} \sum_{\substack{h\in\mathbb{Z}\setminus\{0\}\\ h\equiv_{n/p}-(c/p)z}} \frac{C_{2,d+1}^{\lambda}}{|h|^{2r_{2,d+1}\lambda}} \\
&\le p^{-2r_{2,d+1}\lambda} p \sum_{z=1}^{n/p-1} \sum_{\substack{h\in\mathbb{Z}\setminus\{0\}\\ h\equiv_{n/p} z}} \frac{C_{2,d+1}^{\lambda}}{|h|^{2r_{2,d+1}\lambda}} \\
&= C_{2,d+1}^{\lambda} p^{1-2r_{2,d+1}\lambda} \left(2\zeta(2r_{2,d+1}\lambda) - \frac{2\zeta(2r_{2,d+1}\lambda)}{(n/p)^{2r_{2,d+1}\lambda}}\right) \\
&\le 2C_{2,d+1}^{\lambda}\zeta(2r_{2,d+1}\lambda)\left(1-\frac{1}{n^{2r_{2,d+1}\lambda}}\right). \qquad (46)
\end{aligned}$$

Note that as $\lambda \in (1/(2r_2), 1]$ and $r_{2,d+1} \ge r_2$, we know that $\zeta(2r_{2,d+1}\lambda) < \infty$ and $p^{1-2r_{2,d+1}\lambda} \le 1$. Since the estimate (46) is independent of c, we can express the remaining factor in (45) as

$$\begin{aligned}
\sum_{c=1}^{n-1} \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\equiv_n c}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C_{2,j}^{\lambda}}{|h_j|^{2r_{2,j}\lambda}} &= \sum_{\substack{\boldsymbol{h}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{v}|-1}\\ \boldsymbol{h}\cdot\boldsymbol{z}_{\mathfrak{v}\setminus\{d+1\}}\not\equiv_n 0}} \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \frac{C_{2,j}^{\lambda}}{|h_j|^{2r_{2,j}\lambda}} \\
&= \prod_{j\in\mathfrak{v}\setminus\{d+1\}} \big(2C_{2,j}^{\lambda}\zeta(2r_{2,j}\lambda)\big) - B.
\end{aligned}$$

Combining these elements back into (44), we obtain

$$\begin{aligned}
T_{d+1,s}^{\lambda}(z_{d+1}^*) \le &\sum_{d+1\in\mathfrak{v}\subseteq\{1:d+1\}} \widetilde{\gamma}_{s,\mathfrak{v}}^{\lambda} \left(\frac{2C_{2,d+1}^{\lambda}\zeta(2r_{2,d+1}\lambda)}{n^{2r_{2,d+1}\lambda}} B \right. \\
&\left. + \frac{2C_{2,d+1}^{\lambda}\zeta(2r_{2,d+1}\lambda)}{\varphi(n)}\left(1-\frac{1}{n^{2r_{2,d+1}\lambda}}\right)\left(\prod_{j\in\mathfrak{v}\setminus\{d+1\}}\big(2C_{2,j}^{\lambda}\zeta(2r_{2,j}\lambda)\big) - B\right)\right) \\
\le &\frac{1}{\varphi(n)} \sum_{d+1\in\mathfrak{v}\subseteq\{1:d+1\}} \widetilde{\gamma}_{s,\mathfrak{v}}^{\lambda} \prod_{j\in\mathfrak{v}} \big(2C_{2,j}^{\lambda}\zeta(2r_{2,j}\lambda)\big), \qquad (47)
\end{aligned}$$

where we dropped all terms involving $B > 0$ since the combined coefficient is clearly negative. The required error bound for $E_{d+1,s}^2(z_1^*, \ldots, z_d^*, z_{d+1}^*)$ can now

be obtained by substituting (47) and the induction hypothesis (42) into (43), and then applying Jensen's inequality. By induction we conclude that (42) holds for all $d \in \{1:s\}$. This completes the proof. □

Theorem 8 *Suppose that f belongs to the anchored or unanchored space for some weight parameters $\gamma_{s,\mathfrak{u}}$ and weight functions ψ_j, and suppose that (41) holds for constants $C_{2,j} > 0$ and $r_{2,j} \geq r_2 > 1/2$. Then a generating vector $\boldsymbol{z}^* \in \mathcal{Z}_n^s$ for a randomly-shifted lattice rule can be constructed by a CBC algorithm such that, for all $\lambda \in (1/(2r_2), 1]$,*

$$\begin{aligned}
&\sqrt{\mathbb{E}^{\boldsymbol{\Delta}} |I_{s,\phi}(f) - Q_{s,n}(f \circ \Phi^{-1})|^2} \\
&\leq \left(\frac{1}{\varphi(n)} \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{s,\mathfrak{u}}^{\lambda} \prod_{j \in \mathfrak{u}} \left(C_{0,j}^{\lambda} + 2 C_{2,j}^{\lambda} \zeta(2 r_{2,j} \lambda) \right) \right)^{1/(2\lambda)} \|f\|_{\mathcal{F}}, \qquad (48)
\end{aligned}$$

where the expectation is taken with respect to the random shift which is uniformly distributed on $[0,1]^s$, and $C_{0,j}$ is given by (19) for the anchored variant and $C_{0,j} = 0$ for the unanchored variant.

Proof. From (13) and (14) we see that

$$\begin{aligned}
\mathbb{E}^{\boldsymbol{\Delta}} |I_{s,\phi}(f) - Q_{s,n}(f \circ \Phi^{-1})|^2 &\leq \int_{[0,1]^s} [e^{\mathrm{wor}}(Q_{s,n}; \mathcal{G})]^2 \, \|f\|_{\mathcal{F}}^2 \, \mathrm{d}\boldsymbol{\Delta} \\
&= [e_{s,n}^{\mathrm{sh}}(\boldsymbol{z})]^2 \, \|f\|_{\mathcal{F}}^2.
\end{aligned}$$

Substituting (37) into (42) and applying Jensen's inequality, we obtain

$$\begin{aligned}
[e_{s,n}^{\mathrm{sh}}(\boldsymbol{z}^*)]^2 &= E_{s,s}^2(\boldsymbol{z}^*) \\
&\leq \left(\frac{1}{\varphi(n)} \sum_{\emptyset \neq \mathfrak{v} \subseteq \{1:s\}} \sum_{\mathfrak{v} \subseteq \mathfrak{u} \subseteq \{1:s\}} \gamma_{s,\mathfrak{u}}^{\lambda} \Big(\prod_{j \in \mathfrak{u} \setminus \mathfrak{v}} C_{0,j}^{\lambda} \Big) \prod_{j \in \mathfrak{v}} \left(2 C_{2,j}^{\lambda} \zeta(2 r_{2,j} \lambda) \right) \right)^{1/\lambda} \\
&= \left(\frac{1}{\varphi(n)} \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{s,\mathfrak{u}}^{\lambda} \sum_{\mathfrak{v} \subseteq \mathfrak{u}} \Big(\prod_{j \in \mathfrak{u} \setminus \mathfrak{v}} C_{0,j}^{\lambda} \Big) \prod_{j \in \mathfrak{v}} \left(2 C_{2,j}^{\lambda} \zeta(2 r_{2,j} \lambda) \right) \right)^{1/\lambda},
\end{aligned}$$

which equals the square of the first factor in (48). □

The CBC construction and error bound we have presented thus far depend on the final dimension s. If the weights are independent of s, i.e., $\gamma_{s,\mathfrak{u}} = \gamma_{\mathfrak{u}}$, and if

$$\sum_{|\mathfrak{u}| < \infty} \gamma_{\mathfrak{u}}^{\lambda} \prod_{j \in \mathfrak{u}} \left(C_{0,j}^{\lambda} + 2 C_{2,j}^{\lambda} \zeta(2 r_{2,j} \lambda) \right) < \infty, \qquad (49)$$

then for every s the CBC algorithm yields a generating vector $\boldsymbol{z}^*$ for which $e_{s,n}^{\mathrm{sh}}(\boldsymbol{z}^*) = \mathcal{O}(n^{-1/(2\lambda)})$, with the implied constant independent of s. If the

weights are of a product form, i.e., $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$, then the condition (49) simplifies to $\sum_{j=1}^{\infty} \gamma_j^{\lambda} < \infty$, as seen in earlier papers.

In the unanchored space with weights $\gamma_{\mathfrak{u}}$ independent of s, since there is no need for auxiliary weights (we have $C_{0,j} = 0$ and $\widetilde{\gamma}_{s,\mathfrak{v}} = \gamma_{\mathfrak{v}}$), the CBC algorithm actually works directly with $[e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2$, and the resulting generating vector is *extensible* in dimension. That is, if we have a $\boldsymbol{z} \in \mathcal{Z}_n^s$ constructed using the CBC algorithm, we may re-use $\boldsymbol{z}$ and minimise $[e^{\mathrm{sh}}_{s+1,n}(\boldsymbol{z}, z_{s+1})]^2$ for some z_{s+1}, and we do not have to rebuild the whole generating vector from the bottom up. For general non-product weights $\gamma_{\mathfrak{u}}$, the cost of the CBC algorithm can be prohibitively expensive. In Section 5.2 we will discuss the fast CBC implementation for POD weights (4).

In the anchored space, however, for Theorem 7 to be valid the CBC algorithm must work with the auxiliary quantity $E^2_{d,s}(\boldsymbol{z})$ which involves the auxiliary weights $\widetilde{\gamma}_{s,\mathfrak{v}}$. Even if the original weights $\gamma_{\mathfrak{u}}$ are independent of s, the auxiliary weights $\widetilde{\gamma}_{s,\mathfrak{v}}$ needed in the CBC construction still depend on s by definition, see (37). Thus the resulting generating vector is *not extensible* in dimension, even though the error bound can be independent of s when (49) holds. This means that unique generating vectors $\boldsymbol{z} \in \mathcal{Z}_n^s$ must be built from the bottom up for each s, using the CBC construction. We stress that an implementation based on minimizing $[e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2$ in each step, although intuitively sound, cannot be justified by Theorem 7. Unfortunately, even if the original weights have some nice structure such as POD weights, this structure is not preserved by the auxiliary weights. A method of tackling this issue for the anchored space with POD weights will be discussed Section 5.2.

4.3. Examples of ψ_j and ϕ

In [31] a study is undertaken for various combinations of the weight function ψ_j and probability density ϕ. In particular it is examined whether condition (9) is satisfied, and then rates of decay of $\widehat{\theta}_j(h)$ are calculated.

We present in Table 1 a summary of the condition (9) as well as estimates of $r_{2,j}$ for selected combinations of ϕ and ψ_j. Full details of these calculations can be found in [31], with the exception that the cases with $\psi_j(y) = 1$ are given in [39]. The asterisks in $r^*_{2,j}$ in Table 1 mark those cases where matching lower bounds on $\widehat{\theta}_j(h)$ have been obtained (up to $\delta > 0$), indicating that those estimates on $r_{2,j}$ are sharp.

5. Implementing the CBC algorithm

5.1. Computing θ_j

In order to be able to compute the shift-averaged worst-case error given by (24) or (35), we must be able to compute $\theta_j(i/n)$ as defined in (23), (31) or (32) for $i = 0, \ldots, n-1$. For simplicity we consider here the domain $D = \mathbb{R}$ and

Table 1: Consider selected combinations of the probability density ϕ and weight function ψ_j. Does condition (9) hold? What are the estimates for $r_{2,j}$? The asterisk in $r^*_{2,j}$ below indicates a sharp estimate of $r_{2,j}$.

$\phi(y)$ / $\psi_j(y)$	$\frac{e^{-y^2/2\nu}}{\sqrt{2\pi\nu}}$	$\frac{e^{y/\nu}}{\nu(1+e^{y/\nu})^2}$ or $\frac{e^{-\lvert y\rvert/\nu}}{2\nu}$	$\frac{1}{\sqrt{\nu\pi}}\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}(1+\frac{y^2}{\nu})^{-\frac{\nu+1}{2}}$ or $\frac{\nu}{2}(1+\lvert y\rvert)^{-(\lvert\nu\rvert+1)}$
$e^{-y^2/(2\alpha)}$	Yes if $\alpha > 2\nu$ $r_{2,j} = 1 - \frac{\nu}{\alpha}$	-	-
$e^{-\lvert y\rvert/\alpha}$	Yes $r_{2,j} = 1-\delta,\ \forall\delta \in (0,\frac{1}{2})$	Yes if $\alpha > 2\nu$ $r^*_{2,j} = 1 - \frac{\nu}{\alpha}$	-
$(1+\lvert y\rvert)^{-\alpha}$	Yes $r_{2,j} = 1-\delta,$ $\forall\delta \in (0, \min(\frac{1}{2}, \frac{9}{8}\alpha\nu))$	Yes $r^*_{2,j} = 1-\delta,$ $\forall\delta \in (0, \min(\frac{1}{2}, \alpha\nu))$	Yes if $2\alpha+1 < \nu$ $r^*_{2,j} = 1 - \frac{2\alpha+1}{2\nu}$
1	Yes $r_{2,j} = 1-\delta,\ \forall\delta \in (0,\frac{1}{2})$	Yes $r^*_{2,j} = 1-\delta,\ \forall\delta \in (0,\frac{1}{2})$	Yes if $\nu > 1$ $r^*_{2,j} = 1 - \frac{1}{2\nu}$

anchor $c = 0$. We also assume that ϕ and ψ_j are symmetric about 0. Thus, for the unanchored space we see that for $i \le \lfloor n/2 \rfloor$, (32) becomes

$$\begin{aligned}\theta_j\big(\tfrac{i}{n}\big) \;&=\; 2\int_{\Phi^{-1}(i/n)}^{0} \frac{\Phi(t) - i/n}{\psi_j^2(t)}\,\mathrm{d}t - 2\int_{-\infty}^{0}\frac{\Phi^2(t)}{\psi_j^2(t)}\,\mathrm{d}t \\ &=\; 2\int_{i/n}^{1/2} \frac{x - i/n}{\psi_j^2(\Phi^{-1}(x))\,\phi(\Phi^{-1}(x))}\,\mathrm{d}x - 2\int_0^{1/2}\frac{x^2}{\psi_j^2(\Phi^{-1}(x))\,\phi(\Phi^{-1}(x))}\,\mathrm{d}x,\end{aligned} \tag{50}$$

where we used the substitution $x = \Phi(t)$. We also have $C_{0,j} = 0$ and $C_{1,j} = \theta_j(0)$. For $i > \lfloor n/2 \rfloor$, we use $\theta_j(i/n) = \theta_j((n-i)/n)$ due to symmetry.

The integrals in (50) may now be computed using a one-dimensional quadrature. However, there is a singularity at $x = 0$ for both integrands, thus we make use of the tanh-sinh transform first proposed in [43], see also [3, 4]. For the first integral in (50) we use the substitution

$$x \;=\; v(t) \;=\; \left(\frac{1}{2} - \frac{i}{n}\right)\tanh\left(\frac{\pi}{2}\sinh(t)\right) + \frac{1}{2}.$$

which maps the interval $(-\infty, 0]$ to $(i/n, 1/2]$. A similar substitution can be used for the second integral. We then approximate the integrals with the sum $h\sum_{k=-m}^{0}\Upsilon(v(kh))v'(kh)$, where $\Upsilon(t)$ is our integrand, m is the number of quadrature points, and h is the mesh-size which is chosen here to be $h = \frac{2}{m}\log(\pi m)$ to balance the truncation and discretization errors (see [34] for details). Note that $v(-t) = -v(t)$, so indeed the sum approximates the transformed integral on the half real line $(-\infty, 0]$.

This quadrature for calculating θ_j, $C_{0,j}$ and $C_{1,j}$ evidently requires $\mathcal{O}(m\,n)$ operations. We must choose m to balance the the quadrature error with other sources of error. In general, we may also need to approximate Φ^{-1} numerically.

5.2. Fast CBC construction for POD weights in the unanchored space

Implementation of the CBC construction as described in Algorithm 6 is infeasible unless some structures are assumed for the weights $\gamma_{\mathfrak{u}}$. For product weights $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$, a fast CBC implementation based on FFT is known from [37, 38], which requires only $\mathcal{O}(s\,n\log n)$ operations and $\mathcal{O}(n)$ memory. For order-dependent weights $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}$, a similar fast CBC implementation is discussed in [8], which requires $\mathcal{O}(s\,n\log n + s^2\,n)$ operations and $\mathcal{O}(s\,n)$ memory. The CBC implementation for POD weights (4) is presented in [27] and has the same cost as order-dependent weights.

Here we present a refinement of the strategy from [27] to avoid numerical overflow when the order-dependent parts of POD weights grow very quickly. This consideration is motivated by the form of POD weights which arise from the application to PDEs with random coefficients, see [28],

$$\gamma_{\mathfrak{u}} \;=\; (|\mathfrak{u}|!)^a \prod_{j\in\mathfrak{u}} \gamma_j, \qquad a > 0. \tag{51}$$

That is, we have POD weights (4) where $\Gamma_{|\mathfrak{u}|} = (|\mathfrak{u}|!)^a$. In general, rather than working directly with the sequence $\{\Gamma_\ell\}_{\ell\ge 0}$ in the CBC construction, we shall work with their ratios

$$\alpha_\ell \;:=\; \frac{\Gamma_\ell}{\Gamma_{\ell-1}}, \quad \text{so that} \quad \Gamma_\ell = \prod_{i=1}^{\ell} \alpha_i. \tag{52}$$

Thus in the particular case (51) we have $\alpha_\ell = \ell^a$.

For the unanchored space there are no auxiliary weights, and we have $E^2_{d,s}(\boldsymbol{z}) = [e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2$. At each step of the CBC algorithm we consider the shift-averaged worst-case error $e^{\mathrm{sh}}_{d+1,n}(\boldsymbol{z}, z_{d+1})$ to be a function of z_{d+1}, with $\boldsymbol{z}$ fixed, and for simplicity we write $e^2_{d+1}(z_{d+1}) = [e^{\mathrm{sh}}_{d+1,n}(\boldsymbol{z}, z_{d+1})]^2$. Substituting POD weights

(4) into (35) and using (52), we have

$$
\begin{aligned}
e^2_{d+1}(z_{d+1}) \;&=\; \frac{1}{n}\sum_{k=1}^{n}\sum_{\ell=1}^{d+1}\sum_{\substack{\mathfrak{u}\subseteq\{1:d+1\}\\|\mathfrak{u}|=\ell}}\Big(\prod_{i=1}^{\ell}\alpha_i\Big)\Big(\prod_{j\in\mathfrak{u}}\gamma_j\,\theta_j\Big(\Big\{\frac{kz_j}{n}\Big\}\Big)\Big)\\
&=\; \frac{1}{n}\sum_{k=1}^{n}\sum_{\ell=1}^{d+1}\Bigg(\underbrace{\sum_{\substack{\mathfrak{u}\subseteq\{1:d\}\\|\mathfrak{u}|=\ell}}\Big(\prod_{i=1}^{\ell}\alpha_i\Big)\Big(\prod_{j\in\mathfrak{u}}\gamma_j\,\theta_j\Big(\Big\{\frac{kz_j}{n}\Big\}\Big)\Big)}_{q_{d,\ell}(k)}\\
&\qquad\qquad +\,\gamma_{d+1}\alpha_\ell\,\theta_{d+1}\Big(\Big\{\frac{kz_{d+1}}{n}\Big\}\Big)\underbrace{\sum_{\substack{\mathfrak{u}\subseteq\{1:d\}\\|\mathfrak{u}|=\ell-1}}\Big(\prod_{i=1}^{\ell-1}\alpha_i\Big)\Big(\prod_{j\in\mathfrak{u}}\gamma_j\,\theta_j\Big(\Big\{\frac{kz_j}{n}\Big\}\Big)\Big)}_{q_{d,\ell-1}(k)}\Bigg)\\
&=\; [e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2 \;+\; \frac{\gamma_{d+1}}{n}\sum_{k=1}^{n}\theta_{d+1}\Big(\Big\{\frac{kz_{d+1}}{n}\Big\}\Big)\sum_{\ell=1}^{d+1}\alpha_\ell\,q_{d,\ell-1}(k).
\end{aligned}
$$

We deduce the following recursions to compute $q_{d,\ell}(k)$

$$
\begin{aligned}
q_{d,0}(k) \;&:=\; 1,\\
q_{d+1,\ell}(k) \;&:=\; q_{d,\ell}(k) + \gamma_{d+1}\,\alpha_\ell\,\theta_{d+1}\Big(\Big\{\frac{kz_{d+1}}{n}\Big\}\Big)\,q_{d,\ell-1}(k),
\end{aligned}
\tag{53}
$$

with $q_{d,\ell}(k) := 0$ if $\ell > d$ or $\ell < 0$. We need to evaluate $e^2_{d+1}(z_{d+1})$ for all $z_{d+1} \in \mathcal{Z}_n$. This suggests a matrix-vector operation, where we have the vectors

$$
\boldsymbol{e}^2_{d+1} \;:=\; [e^2_{d+1}(z)]_{z\in\mathcal{Z}_n}, \quad \boldsymbol{q}_{d,\ell} \;:=\; [q_{d,\ell}(k)]_{1\le k\le n},
\tag{54}
$$

and the matrix

$$
\boldsymbol{\Omega}_{n,d+1} \;:=\; \Big[\theta_{d+1}\Big(\Big\{\frac{kz}{n}\Big\}\Big)\Big]_{\substack{z\in\mathcal{Z}_n\\1\le k\le n}} \;=\; \Big[\theta_{d+1}\Big(\frac{kz \bmod n}{n}\Big)\Big]_{\substack{z\in\mathcal{Z}_n\\1\le k\le n}}.
\tag{55}
$$

We can now write the calculation of $\boldsymbol{e}^2_{d+1}$ as follows

$$
\boldsymbol{e}^2_{d+1} \;=\; [e^{\mathrm{sh}}_{d,n}(\boldsymbol{z})]^2\,\mathbf{1}_{\varphi(n)} \;+\; \frac{\gamma_{d+1}}{n}\,\boldsymbol{\Omega}_{n,d+1}\Big(\sum_{\ell=1}^{d+1}\alpha_\ell\,\boldsymbol{q}_{d,\ell-1}\Big),
$$

where $\mathbf{1}_{\varphi(n)}$ is a vector of ones of length $\varphi(n)$ (i.e., with as many elements as there are rows in $\boldsymbol{\Omega}_{n,d+1}$). Now we choose the value of $z_{d+1} \in \mathcal{Z}_n$ that corresponds to the the smallest entry in $\boldsymbol{e}^2_{d+1}$. For this crucial step, the key is to permute the rows and columns of the matrix $\boldsymbol{\Omega}_{n,d+1}$ so that it becomes a circulant (or block-circulant-with-circulant-blocks) matrix (except for the column

of zeros corresponding to $k = n$), enabling us to perform fast matrix-vector multiplications using FFT methods, for details see [37, 38, 8].

The next step is to generate the vectors $\boldsymbol{q}_{d+1,\ell}$ for each $\ell = 1, \ldots, d+1$ using the formula

$$\boldsymbol{q}_{d+1,\ell} \;=\; \boldsymbol{q}_{d,\ell} + \gamma_{d+1}\,\alpha_\ell\,\boldsymbol{\Omega}^P_{n,d+1}(z_{d+1}) \;.*\; \boldsymbol{q}_{d,\ell-1},$$

where $\boldsymbol{\Omega}^P_{n,d+1}(z_{d+1})$ is the row of the permuted matrix $\boldsymbol{\Omega}^P_{n,d+1}$ that corresponds to the chosen z_{d+1}, and the operator $.*$ denotes element-wise vector-vector multiplication. We see that we must maintain storage of the vectors $\boldsymbol{q}_{d+1,\ell}$ for $\ell = 1, \ldots, d$ at each iteration $d+1$, however we can overwrite $\boldsymbol{q}_{d,\ell}$ with $\boldsymbol{q}_{d+1,\ell}$ at each step, hence we require $\mathcal{O}(s\,n)$ storage for the algorithm. Note that there is no need to permute the vectors $\boldsymbol{q}_{d+1,\ell}$ since in the first dimension all components are initialized to the same value 1.

Therefore this procedure has a "search" cost of $\mathcal{O}(n \log n)$ operations which corresponds to the use of FFT for the matrix-vector multiplication, and there is an "update" cost of $\mathcal{O}(d\,n)$ operations at step d which is needed for calculating the vectors $\boldsymbol{q}_{d,\ell}$. The overall construction cost is therefore

$$\sum_{d=1}^{s} \mathcal{O}(n \log n + d\,n) \;=\; \mathcal{O}(s\,n \log n + s^2 n) \quad \text{operations.}$$

5.3. Fast CBC construction for POD weights in the anchored space

For the anchored space, POD weights are not preserved by the auxiliary weights which are used for the implementation of the CBC algorithm, making the computational cost prohibitive. A remedy has been proposed in [15] for POD weights of the special form (51) which arise from PDE applications. The corresponding auxiliary weights (37) can be bounded as follows

$$\begin{aligned}
\widetilde{\gamma}_{s,\mathfrak{v}} \;&=\; \sum_{\mathfrak{v}\subseteq\mathfrak{u}\subseteq\{1:s\}} (|\mathfrak{u}|!)^a \left(\prod_{j\in\mathfrak{u}} \gamma_j\right)\left(\prod_{j\in\mathfrak{u}\setminus\mathfrak{v}} C_{0,j}\right) \\
&=\; (|\mathfrak{v}|!)^a \left(\prod_{j\in\mathfrak{v}} \gamma_j\right) \sum_{\mathfrak{w}\subseteq\{1:s\}\setminus\mathfrak{v}} \left(\frac{(|\mathfrak{v}|+|\mathfrak{w}|)!}{|\mathfrak{v}|!}\right)^a \prod_{j\in\mathfrak{w}} (C_{0,j}\,\gamma_j) \\
&\le\; (|\mathfrak{v}|!)^a \left(\prod_{j\in\mathfrak{v}} \gamma_j\right) \sum_{\mathfrak{w}\subseteq\{1:s\}\setminus\mathfrak{v}} \left(|\mathfrak{w}|!\,2^{|\mathfrak{v}|+|\mathfrak{w}|}\right)^a \prod_{j\in\mathfrak{w}} (C_{0,j}\,\gamma_j) \;\le\; \widetilde{\widetilde{\gamma}}_{\mathfrak{v}}\, c_{s,\boldsymbol{\gamma}},
\end{aligned}$$

where

$$\widetilde{\widetilde{\gamma}}_{\mathfrak{v}} \;:=\; (|\mathfrak{v}|!)^a \prod_{j\in\mathfrak{v}} (2^a\,\gamma_j) \quad \text{and} \quad c_{s,\boldsymbol{\gamma}} \;:=\; \sum_{\mathfrak{w}\subseteq\{1:s\}} (|\mathfrak{w}|!)^a \prod_{j\in\mathfrak{w}} (2^a\,C_{0,j}\,\gamma_j).$$

Using this we can see, from (38) and the steps in the proof of Lemma 4, that

$$[e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})]^2 \;\le\; c_{s,\boldsymbol{\gamma}} \sum_{\emptyset\ne\mathfrak{v}\subseteq\{1:s\}} \frac{\widetilde{\widetilde{\gamma}}_{\mathfrak{v}}}{n} \sum_{k=1}^{n} \prod_{j\in\mathfrak{v}} \left(\theta_j\left(\left\{\frac{k z_j}{n}\right\}\right) - C_{0,j}\right).$$

The expression on the right-hand side, without the $c_{s,\boldsymbol{\gamma}}$ factor, can be used as the search criterion in the CBC algorithm and we can obtain a similar error bound as Theorem 7. Since the new weights $\widetilde{\widetilde{\gamma}}_{\mathfrak{v}}$ are of POD form, the algorithm can be implemented as in the case for the unanchored space.

6. Numerical experiments

We implement the CBC algorithm in the unanchored space with POD weights given by

$$\gamma_{s,\mathfrak{u}} = \gamma_{\mathfrak{u}} = \left((|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} \frac{\kappa}{j^\eta}\right)^{1/(1+\lambda)},$$

for some $\kappa > 0$, $\eta > 2$, and $1/2 < \lambda \le 1$. This choice of weights is inspired by the form of the weights derived in [22]. We consider three combinations of probability densities ϕ and weight functions $\psi_j = \psi$:

Combination 1 $\phi(y) = e^{-x^2/2}/\sqrt{2\pi}$ and $\psi(y) = e^{-|x|/\alpha}$.

Combination 2 $\phi(y) = e^{-x^2/2}/\sqrt{2\pi}$ and $\psi(y) = e^{-x^2/(2\alpha)}$.

Combination 3 $\phi(y) = e^{-|x|}/2$ and $\psi(y) = 1$.

In particular, we take a selection of parameters

$$\eta = 3.1,\, 5.0, \quad \kappa = 0.01,\, 0.1, \quad \lambda = 0.51,\, 0.75 \quad \text{and} \quad \alpha = 4,\, 16,$$

and implement the CBC algorithm for $n = 1009, 2003, 4001, 8009, 16001, 32003$, up to $s = 100$ dimensions. For the numerical computation of θ_j, we set the parameter $m = 1000$, which appears to provide a reasonable accuracy for θ_j. The corresponding shift-averaged worst-case errors $e^{\mathrm{sh}}_{s,n}(\boldsymbol{z})$ are presented in Tables 2–6, together with an estimate on the observed rate of convergence $\mathcal{O}(n^{-r})$, found by performing a linear-least squares fit on the log-log plot of the results.

Table 2: $e_{s,n}^{\mathrm{sh}}$ for Combination 1, $\lambda = 0.51$

	$\eta = 3.1$				$\eta = 5$			
	$\alpha = 4$		$\alpha = 16$		$\alpha = 4$		$\alpha = 16$	
n	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$
1009	5.73e-04	2.71e-03	4.59e-04	2.12e-03	3.76e-04	1.06e-03	3.05e-04	8.44e-04
2003	3.14e-04	1.63e-03	2.48e-04	1.26e-03	1.97e-04	5.72e-04	1.58e-04	4.49e-04
4001	1.71e-04	9.63e-04	1.33e-04	7.31e-04	1.03e-04	3.11e-04	8.21e-05	2.41e-04
8009	9.36e-05	5.74e-04	7.21e-05	4.31e-04	5.40e-05	1.68e-04	4.25e-05	1.29e-04
16001	5.12e-05	3.43e-04	3.89e-05	2.52e-04	2.82e-05	9.08e-05	2.19e-05	6.84e-05
32003	2.83e-05	2.04e-04	2.12e-05	1.49e-04	1.47e-05	4.91e-05	1.14e-05	3.66e-05
r	0.869	0.749	0.888	0.766	0.937	0.887	0.950	0.906

Table 3: $e_{s,n}^{\mathrm{sh}}$ for Combination 1, $\lambda = 0.75$

	$\eta = 3.1$				$\eta = 5$			
	$\alpha = 4$		$\alpha = 16$		$\alpha = 4$		$\alpha = 16$	
n	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$
1009	1.05e-03	5.03e-03	8.33e-04	3.93e-03	5.25e-04	1.48e-03	4.23e-04	1.17e-03
2003	6.00e-04	3.14e-03	4.71e-04	2.42e-03	2.79e-04	8.20e-04	2.22e-04	6.38e-04
4001	3.38e-04	1.92e-03	2.62e-04	1.46e-03	1.48e-04	4.57e-04	1.17e-04	3.48e-04
8009	1.93e-04	1.18e-03	1.48e-04	8.87e-04	7.86e-05	2.53e-04	6.11e-05	1.92e-04
16001	1.10e-04	7.33e-04	8.31e-05	5.42e-04	4.16e-05	1.40e-04	3.20e-05	1.04e-04
32003	6.33e-05	4.53e-04	4.72e-05	3.31e-04	2.19e-05	7.72e-05	1.67e-05	5.70e-05
r	0.808	0.697	0.827	0.715	0.917	0.853	0.933	0.872

Table 4: $e_{s,n}^{\mathrm{sh}}$ for Combination 2, $\lambda = 0.51$

	$\eta = 3.1$				$\eta = 5$			
	$\alpha = 4$		$\alpha = 8$		$\alpha = 4$		$\alpha = 8$	
n	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$
1009	1.04e-03	3.96e-03	6.14e-04	2.63e-03	7.63e-04	1.95e-03	4.24e-04	1.14e-03
2003	6.10e-04	2.44e-03	3.40e-04	1.57e-03	4.41e-04	1.14e-03	2.29e-04	6.24e-04
4001	3.57e-04	1.49e-03	1.87e-04	9.29e-04	2.55e-04	6.65e-04	1.23e-04	3.44e-04
8009	2.09e-04	9.16e-04	1.04e-04	5.56e-04	1.47e-04	3.89e-04	6.63e-05	1.90e-04
16001	1.22e-04	5.63e-04	5.75e-05	3.30e-04	8.54e-05	2.28e-04	3.57e-05	1.04e-04
32003	7.18e-05	3.47e-04	3.21e-05	1.98e-04	4.95e-05	1.33e-04	1.92e-05	5.75e-05
r	0.773	0.704	0.853	0.748	0.790	0.775	0.894	0.862

Table 5: $e_{s,n}^{\mathrm{sh}}$ for Combination 2, $\lambda = 0.75$

	$\eta = 3.1$				$\eta = 5$			
	$\alpha = 4$		$\alpha = 8$		$\alpha = 4$		$\alpha = 8$	
n	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$
1009	1.70e-03	6.79e-03	1.07e-03	4.72e-03	1.03e-03	2.56e-03	5.82e-04	1.55e-03
2003	1.01e-03	4.30e-03	6.11e-04	2.93e-03	5.96e-04	1.50e-03	3.16e-04	8.62e-04
4001	5.99e-04	2.70e-03	3.46e-04	1.79e-03	3.46e-04	8.88e-04	1.71e-04	4.85e-04
8009	3.58e-04	1.70e-03	1.99e-04	1.10e-03	2.01e-04	5.26e-04	9.33e-05	2.71e-04
16001	2.14e-04	1.08e-03	1.14e-04	6.79e-04	1.17e-04	3.10e-04	5.06e-05	1.52e-04
32003	1.28e-04	6.81e-04	6.57e-05	4.20e-04	6.79e-05	1.83e-04	2.74e-05	8.52e-05
r	0.747	0.665	0.805	0.699	0.785	0.761	0.882	0.837

Table 6: $e^{\text{sh}}_{s,n}$ for Combination 3

	$\lambda = 0.51$				$\lambda = 0.75$			
	$\eta = 3.1$		$\eta = 5$		$\eta = 3.1$		$\eta = 5$	
n	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$	$\kappa = 0.01$	$\kappa = 0.1$
1009	6.91e-04	3.30e-03	4.49e-04	1.29e-03	1.26e-03	6.08e-03	6.31e-04	1.81e-03
2003	3.82e-04	2.01e-03	2.37e-04	7.02e-04	7.29e-04	3.83e-03	3.38e-04	1.01e-03
4001	2.12e-04	1.20e-03	1.25e-04	3.86e-04	4.17e-04	2.37e-03	1.81e-04	5.66e-04
8009	1.16e-04	7.21e-04	6.57e-05	2.11e-04	2.40e-04	1.48e-03	9.66e-05	3.19e-04
16001	6.42e-05	4.34e-04	3.44e-05	1.15e-04	1.39e-04	9.20e-04	5.14e-05	1.78e-04
32003	3.59e-05	2.63e-04	1.82e-05	6.27e-05	8.05e-05	5.79e-04	2.75e-05	9.96e-05
r	0.855	0.733	0.925	0.872	0.793	0.681	0.904	0.837

The numbers presented demonstrate that our theory holds reasonably well, however, there is a strong dependency on certain parameters of the weights. We focus our attention primarily on the rate of convergence.

The parameter κ does not affect the theoretical convergence rate, but it has a strong effect on the scaling of $e^{\text{sh}}_{s,n}$. This is evident when one considers higher-order weights (i.e., weights $\gamma_{\mathfrak{u}}$ with large cardinality $|\mathfrak{u}|$), as there is a factor of $\kappa^{|\mathfrak{u}|}$ in the weights. For larger κ, the constant factor in the error bound can be quite large, and we may not observe the theoretical convergence rate with small to moderate values of n.

The parameter α may affect the theoretical convergence rate, as seen in Table 1. Combination 3 has no parameter α, and for Combination 1 there is no theoretical dependence of the convergence rate on α. In both cases the theoretical convergence rate is $\mathcal{O}(n^{-1+\delta})$ for any $\delta > 0$, provided we take the choice of $\lambda = 1/(2-2\delta)$. In the numerics this is mostly reflected, and we see that there is a much stronger dependence on η and κ than on α. For Combination 2, however, while we do not observe precisely the theoretical rate of $1 - 1/\alpha$, there is a noticeable dependence of the observed rate on α.

Finally, we observe that the parameter η does not have an explicit impact on the rates of convergence for a fixed s. However it does have an impact on the condition (49), and hence affects implicitly what range of λ are possible if we want our bound of $e^{\text{sh}}_{s,n}$ to be independent of s. In any case, we see that η affects the scaling of $e^{\text{sh}}_{s,n}$.

Acknowledgement

The support of the Australian Research Council is gratefully acknowledged. The authors thank Ian Sloan, Grzegorz Wasilkowski, Stephen Joe, and the referees for valuable comments and suggestions.

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