Covering of spheres by spherical caps and worst-case error for equal weight cubature in Sobolev spaces [☆]

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A R T I C L E   I N F O

A B S T R A C T

We prove that the covering radius of an N-point subset X_N of the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ is bounded above by a power of the worst-case error for equal weight cubature $\frac{1}{N} \sum_{\mathbf{x} \in X_N} f(\mathbf{x}) \approx \int_{\mathbb{S}^d} f \, d\sigma_d$ for functions in the Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$, where σ_d denotes normalized area measure on $\mathbb{S}^d$. These bounds are close to optimal when s is close to d/p. Our study of the worst-case error along with results of Brandolini et al. motivate the definition of Quasi-Monte Carlo (QMC) design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$, which have previously been introduced only in the Hilbert space setting $p = 2$. We say that a sequence (X_N) of N-point configurations is a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$ with $s > d/p$ provided the worst-case equal weight cubature error for X_N has order $N^{-s/d}$ as $N \to \infty$, a property that holds, in particular, for a sequence of spherical t-designs in which each design has order t^d points. For the case $p = 1$, we deduce that any QMC-design sequence (X_N) for $\mathbb{W}_1^s(\mathbb{S}^d)$ with $s > d$ has the optimal covering property; i.e., the covering radius of X_N has order $N^{-1/d}$ as $N \to \infty$. A significant portion of our effort is devoted to the formulation of the worst-case error in terms of a Bessel kernel, and showing that this kernel satisfies a Bernstein type inequality involving the mesh ratio of X_N. As a consequence we prove that any QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$ is also a QMC-design sequence for $\mathbb{W}_{p'}^s(\mathbb{S}^d)$ for all $1 \leq p < p' \leq \infty$ and, furthermore, if (X_N) is a quasi-uniform QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$, then it is also a QMC-design sequence for $\mathbb{W}_p^{s'}(\mathbb{S}^d)$ for all $s > s' > d/p$.

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1. Introduction

In this paper we consider covering the unit sphere $\mathbb{S}^d$ in $\mathbb{R}^{d+1}$, $d \geq 1$, with equal sized spherical caps, and establish a connection to equal weight cubature formulas that use the centers of those caps as sampling points for the function. As a corollary, we will show that the optimal order of convergence of the worst-case equal weight cubature error for functions in a suitable Sobolev space implies asymptotically an optimal covering property by spherical caps.

Equal-weight numerical integration In the literature equal weight cubature is often given the name Quasi-Monte Carlo (see Niederreiter [24] for the case of the unit cube). Thus a *Quasi-Monte Carlo (QMC) method* is an equal weight numerical integration formula with *deterministic* node set in contrast to Monte Carlo methods: for a node set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$, the QMC method

$$\mathrm{Q}[X_N](f) := \frac{1}{N} \sum_{k=1}^{N} f(\mathbf{x}_k)$$

is a natural approximation of the integral

$$\mathrm{I}(f) := \int_{\mathbb{S}^d} f(\mathbf{x}) \mathrm{d}\sigma_d(\mathbf{x})$$

of a given continuous real-valued function f on $\mathbb{S}^d$ with respect to the normalized surface area measure on $\mathbb{S}^d$. A node set X_N is deterministically chosen in a sensible way so as to guarantee "small" error of numerical integration for functions in suitable subfamilies of the class of continuous functions $C(\mathbb{S}^d)$.

A fundamental example of such node sets are *spherical t-designs*[1] $Z_{N_t} \subset \mathbb{S}^d$, $t \geq 1$, introduced in [10]. They define QMC methods that integrate exactly all spherical polynomials of degree $\leq t$:

$$\mathrm{Q}[Z_{N_t}](P) = \mathrm{I}(P), \qquad \deg P \leq t. \tag{1.1}$$

Thus, spherical t-designs yield zero error on polynomial subfamilies of $C(\mathbb{S}^d)$. The definition of spherical t-designs says nothing about the number of points N_t that might be needed. A lower bound on N_t of order t^d was given in [10]. Recently, Bondarenko et al. [4] proved:

Proposition 1.1. *There exists $c_d > 0$ such that to every $N \geq c_d t^d$ and $t \geq 1$ there exists an N-point spherical t-design on $\mathbb{S}^d$.*

This key result ensures that spherical t-designs with N_t points of exactly the optimal order t^d exist for every $t \geq 1$ (we write $N_t \asymp t^d$). A sequence (Z_{N_t}) of such designs with optimal order for the number of points has the remarkable property, see [8,14], that

$$|\mathrm{Q}[Z_{N_t}](f) - \mathrm{I}(f)| \leq c \, N_t^{-s/d} \, \|f\|_{H^s}$$

for all functions f in a Sobolev space H^s with smoothness index $s > d/2$ and norm $\| \cdot \|_{H^s}$ in the Hilbert space setting. The order of N_t cannot be improved, see [12,13]. This observation motivated the introduction of *QMC-design sequences* for Sobolev spaces H^s in [9]: these are sequences of N-point sets that have the same error behavior as spherical t-designs, but with no polynomial exactness requirement. One purpose of this paper is to provide the extension to general Sobolev spaces.

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[1] The symbol X_N is used for general sets of N points on $\mathbb{S}^d$, while Z_{N_t} always refers to a spherical t-design with N_t points.

Covering for the sphere For a finite set $X_N = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$ *the covering radius* (or *mesh norm*, or *fill radius*) is defined by

$$\rho(X_N) := \max_{\mathbf{x} \in \mathbb{S}^d} \min_{1 \le k \le N} \arccos(\mathbf{x} \cdot \mathbf{x}_k). \tag{1.2}$$

Thus the covering radius is the geodesic radius of the largest hole in the mesh formed by the point set X_N. Equivalently, it is the minimal radius of equal-sized spherical caps centered at the points of X_N that cover $\mathbb{S}^d$. There is a trivial lower bound on $\rho(X_N)$ arising from the fact that a spherical cap of geodesic radius $\rho(X_N)$ has a surface area of exact order $[\rho(X_N)]^d$: it follows that there exists $c_d > 0$ such that

$$\rho(X_N) \ge c_d \, N^{-1/d} \qquad \text{for all } N.$$

We will therefore say that a sequence (X_N) of point sets on $\mathbb{S}^d$ has the *optimal covering property* if

$$\rho(X_N) = \mathcal{O}(N^{-1/d}) \qquad \text{as } N \to \infty. \tag{1.3}$$

Yudin [30] showed that if Z_{N_t} is a spherical t-design, then Z_{N_t} gives a covering of the sphere $\mathbb{S}^d$ with radius $\eta_{t,d}$, where $\cos(\eta_{t,d})$ is the largest zero of a certain Jacobi polynomial. Reimer [25,26] extended Yudin's result to any positive weight cubature rule that is exact for polynomials of degree at most t, and used results relating the largest zero of Gegenbauer polynomials to the first positive zero of a Bessel function, to show that such point sets, which include spherical t-designs, have covering radius $\rho(Z_{N_t}) = \mathcal{O}_d(1/t)$, where the order notation $\mathcal{O}_d$ means that the implied constant depends only on d.

Yudin's result implies that a sequence of spherical t-designs with $N_t \asymp t^d$ points has the optimal covering property (1.3). Reimer's result also shows that the node sets of positive weight cubature rules that are exact for polynomials of degree at most t and have $N = \mathcal{O}_d(t^d)$ points form a sequence that has the optimal covering property. The present paper extends Yudin's result in a different direction, replacing the condition that polynomials of degree up to t be integrated exactly by a condition on the rate of convergence of the QMC error.

The results In this paper the worst-case error will play an important role. For a Banach space B of continuous functions on $\mathbb{S}^d$ with norm $\| \cdot \|_B$, the *worst-case error* for the QMC method $\mathrm{Q}[X_N]$ with node set $X_N \subset \mathbb{S}^d$ approximating the integral $\mathrm{I}(f)$ is defined by

$$\mathrm{wce}(\mathrm{Q}[X_N]; B) := \sup \left\{ \left| \mathrm{Q}[X_N](f) - \mathrm{I}(f) \right| : f \in B, \|f\|_B \le 1 \right\}. \tag{1.4}$$

That is, the worst-case error is the largest error (for the supremum is indeed a maximum) for all functions in the unit ball of B.

We shall be interested in particular in the Sobolev spaces $\mathbb{W}_p^s(\mathbb{S}^d)$ for $p \ge 1$ and $s \ge 0$ consisting of functions $f \in \mathbb{L}_p(\mathbb{S}^d)$ for which $(1 - \Delta_d^*)^{s/2} f \in \mathbb{L}_p(\mathbb{S}^d)$, where Δ_d^* is the Laplace–Beltrami operator on $\mathbb{S}^d$. The Sobolev norm $\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)}$ of f is defined to be the $\mathbb{L}_p(\mathbb{S}^d)$-norm $\|(1 - \Delta_d^*)^{s/2} f\|_p$. For a full description of the Sobolev space setting, see Section 3. We show in Section 4 that the worst-case error of $\mathrm{Q}[X_N]$ for $\mathbb{W}_p^s(\mathbb{S}^d)$ is equal to the $\mathbb{L}_q(\mathbb{S}^d)$-norm (with $1/p + 1/q = 1$) of a function that is related to the Bessel kernel for $\mathbb{W}_p^s(\mathbb{S}^d)$.

A principal result of the paper is that the covering radius of a point set X_N on $\mathbb{S}^d$ is upper bounded by a power of the worst-case error in a Sobolev space:

Theorem 1.2. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ and $s > d/p$. For a positive integer N, let X_N be an N-point set on $\mathbb{S}^d$. Then*

$$\rho(X_N) \leq c_{s,d} \left[\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \right]^{1/(s+d/q)}, \tag{1.5}$$

where the constant $c_{s,d}$ depends on s and d but not on p, q or N.

The theorem will be proved in Section 2. Note that the condition $s > d/p$ is natural, in that it ensures that the generalized Sobolev space is continuously embedded in the space of continuous functions on $\mathbb{S}^d$. The significance of (1.5) is that results on the order of decay of worst-case cubature errors on $\mathbb{S}^d$ as $N \to \infty$ translate directly into bounds for the decay of the covering radius. See Corollary 1.7 below for a concrete instance that ensures optimal order convergence of the covering radius.

The fact that spherical t-designs with $N_t \asymp t^d$ points have optimal order of decay for the worst-case error in Sobolev spaces is a consequence of results due to Brandolini et al. [6], generalizing earlier results for $p = 2$ of [14] and [8]:

Proposition 1.3. *(Cf. [6, Lemma 2.10].) Let $1 \leq p \leq \infty$. Given $s > d/p$, there exists $C_{p,s,d} > 0$ such that for every N-point spherical t-design X_N on $\mathbb{S}^d$ there holds*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq \frac{C_{p,s,d}}{t^s}, \tag{1.6}$$

where the constant $C_{p,s,d}$ does not depend on t, N, or the particular spherical design X_N.

Motivated by Propositions 1.1 and 1.3, we extend the definition of QMC-design sequences as given in [9] from $p = 2$ to general p:

Definition 1.4. *Let $1 \leq p \leq \infty$. Given $s > d/p$, a sequence (X_N) of N-point configurations on $\mathbb{S}^d$ with $N \to \infty$ is a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$ if there exists $c_{p,s,d} > 0$, independent of N, such that*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq \frac{c_{p,s,d}}{N^{s/d}}. \tag{1.7}$$

In this definition it is sufficient that X_N exists for each N in an infinite subset of the natural numbers.

The existence of spherical t-design sequences with $N_t \asymp t^d$ points (Proposition 1.1) and Proposition 1.3 imply the existence of QMC-design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$:

Theorem 1.5 *(Existence of QMC-design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$). For any $1 \leq p \leq \infty$ and $s > d/p$, there exists a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$.*

In particular, any sequence of minimizers of $\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d))$ for a fixed $s > d/p$ and an infinite number of values of N is a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$.

By a special case of [6, Theorem 2.16], which generalizes the earlier $p = 2$ lower bounds of [13] and [12], the exponent of N in (1.7) cannot be larger than s/d:

Proposition 1.6. *Let $1 \leq p \leq \infty$. Given $s > d/p$, there exists $c'_{p,s,d} > 0$ such that for any N-point configuration X_N on $\mathbb{S}^d$,*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \geq \frac{c'_{p,s,d}}{N^{s/d}}. \tag{1.8}$$

Thus a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$ yields error bounds of optimal order of convergence $N^{-s/d}$ for the worst-case error in $\mathbb{W}_p^s(\mathbb{S}^d)$ as $N \to \infty$.

As a consequence of Theorem 1.2, we obtain the following estimate for the covering radius for QMC-design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$, which is sharp when $p = 1$.

Corollary 1.7. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$. For a fixed $s > d/p$, let (X_N) with $N \to \infty$ be a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$. Then there exists a constant $c > 0$ depending on d, s, p and the sequence (X_N) but not on N such that for all X_N*

$$\rho(X_N) \leq c\, N^{-\beta/d}, \qquad \beta := s/(s + d/q).$$

In particular, if $p = 1$ (and thus $\beta = 1$ and $s > d$), then the sequence (X_N) has the optimal covering property.

When $p = 2$, an alternative approach to generating QMC-design sequences is to maximize the generalized sum of distances $\sum_{i=1}^{N} \sum_{j=i}^{N} |\mathbf{x}_i - \mathbf{x}_j|^{2s-d}$. Theorem 14 of [9] shows that such point sets minimize the worst-case error in $\mathbb{W}_2^s(\mathbb{S}^d)$, $s \in (d/2, d/2 + 1)$, and thus form a QMC-design sequence for this Sobolev space.

Example 1.8. Let $d \geq 1$, and for $\alpha \in (0, 2)$ let (X_N) be a sequence of N-point sets such that $X_N \subset \mathbb{S}^d$ is a maximizing set for the generalized sum of distances,

$$\sum_{i=1}^{N} \sum_{j=1}^{N} |\mathbf{x}_i - \mathbf{x}_j|^{\alpha}, \qquad \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \mathbb{S}^d,$$

where $|\cdot|$ denotes Euclidean distance in $\mathbb{R}^{d+1}$. Then setting $p = 2$ in Corollary 1.7, there exists $c > 0$ such that

$$\rho(X_N) \leq cN^{-\beta/d} \qquad \text{with} \qquad \beta = (d + \alpha)/(2d + \alpha).$$

Note that for $d = 2$ the rate approaches $N^{-1/3}$ as $\alpha \to 2^-$ and $N^{-1/4}$ as $\alpha \to 0^+$. Further observe, that the bounds obtained here for any $d \geq 2$ are much better than those derived from using an area bound for the largest spherical cap that contains no points of X_N. The estimates obtained in [21] for $\alpha \in (0, 1)$ and [7] as $\alpha \to 0^+$ yield that the coefficient β above becomes $\beta' = (d + \alpha)/[d(d + 2)]$.

We also obtain the following lower bound on the covering radius:

Theorem 1.9. *Let $d \geq 1$, $1 < p \leq \infty$ with $1/p + 1/q = 1$. For every fixed $s \in (d/p, d)$ there exists a QMC-design sequence (X_N) for $\mathbb{W}_p^s(\mathbb{S}^d)$ such that*

$$\rho(X_N) \geq c'_{p,s,d}\, N^{-s/d^2} \qquad \text{for all } X_N, \tag{1.9}$$

where the constant $c'_{s,d}$ depends on p, s and d but not on N.

For values of p larger than 1 and s a fixed number in $(d/p, d)$, Theorem 1.9 shows that there exists a QMC-design sequence (X_N) for $\mathbb{W}_p^s(\mathbb{S}^d)$ that does *not* have the optimal covering property (1.3) because $s/d^2 < 1/d$.

The next two theorems assert conditions under which a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$ retains the QMC-design property if the parameters p and s are changed. These results are proved in Section 4.2 using lemmas from Sections 5 and 6.

Theorem 1.10. *Let $d \geq 1$, $1 \leq p < \infty$ and $s > d/p$. A QMC-design sequence (X_N) for $\mathbb{W}_p^s(\mathbb{S}^d)$ is also a QMC-design sequence for $\mathbb{W}_{p'}^s(\mathbb{S}^d)$ for all p' satisfying $p < p' \leq \infty$.*

The second theorem makes use of the *mesh ratio*

$$\gamma(X_N) := \rho(X_N)/\delta(X_N) \tag{1.10}$$

of an N-point configuration $X_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^d$, where the *separation distance* of X_N is given by

$$\delta(X_N) := \min_{\substack{1 \leq j,k \leq N \\ j \neq k}} \arccos(\mathbf{x}_j \cdot \mathbf{x}_k). \tag{1.11}$$

A sequence (X_N) of N-point sets on $\mathbb{S}^d$ is *well-separated* if there is a positive constant c such that $\delta(X_N) \geq c\, N^{-1/d}$ and *quasi-uniform* provided $\gamma(X_N)$ is uniformly bounded in N.

Theorem 1.11. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ satisfying $1/p + 1/q = 1$ and $s > s' > d/p$. Then there exists a constant $c > 0$, depending on $p, s', s,$ and d but independent of N, such that for every N-point node set $X_N \subset \mathbb{S}^d$,*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^{s'}(\mathbb{S}^d)) \leq c\, [\gamma(X_N)]^{d/p}\, N^{(s-s')/d}\, \mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)). \tag{1.12}$$

Consequently, a quasi-uniform QMC-design sequence (X_N) for $\mathbb{W}_p^s(\mathbb{S}^d)$ is also a QMC-design sequence for $\mathbb{W}_p^{s'}(\mathbb{S}^d)$ for all s' satisfying $s > s' > d/p$.

A substantial part of the paper is devoted to establishing the estimate (1.12). (Although needed for our argument, it is plausible that the quasi-uniformity assumption in the second assertion of Theorem 1.11 can be removed.)

The structure of the paper is as follows. In the next section we prove Theorems 1.2 and 1.9 and we extend Theorem 1.2 to take into account the radii of several caps excluding points of X_N. In Section 3, we discuss the function space setting and introduce the Bessel kernel for $\mathbb{W}_p^s(\mathbb{S}^d)$. In Section 4, we present a worst-case error formula in terms of a Bessel kernel, which is used to prove embedding type results for QMC-design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$ when p and s vary. In Section 5, we introduce a special filtered kernel that enables us to prove a boundedness result for the Bessel kernel. In Section 6, such filtered kernels are further used to prove a Bernstein type inequality for the Bessel kernel which is needed for the proof of the inequality (1.12). Section 7 considers the special case of the unit circle (i.e., the sphere $\mathbb{S}^1$).

2. Bounds for the covering radius

In this section we give the proofs of Theorems 1.2, and 1.9.

2.1. Upper bound

For the proof of Theorem 1.2 we shall make use of the following interpolation inequality (of Gagliardo–Nirenberg type) on the sphere (see [3]).

Lemma 2.1. *Let $d \geq 1$, $1 \leq p \leq \infty$ and $0 \leq s_0 < s < s_1 < \infty$. Then there exists a constant c depending only on s, p, and d such that for any $0 \leq \theta \leq 1$ and $s = (1-\theta)s_0 + \theta s_1$, we have*

$$\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \leq c\, \|f\|_{\mathbb{W}_p^{s_0}(\mathbb{S}^d)}^{1-\theta}\, \|f\|_{\mathbb{W}_p^{s_1}(\mathbb{S}^d)}^{\theta}. \tag{2.1}$$

Proof of Theorem 1.2. For a node set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ on $\mathbb{S}^d$, we construct a "fooling function" made up of a bump that is supported on a "spherical collar" contained in the largest hole of X_N. The outer radius of this collar is chosen to be $\rho = \rho(X_N)$. The function f_ρ is defined so that it is zero at every point of X_N, thus providing a lower bound for the worst-case error (cf. (1.4)):

$$\text{wce}(Q[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \geq \frac{|\,\mathrm{I}(f_\rho)|}{\|f_\rho\|_{\mathbb{W}_p^s(\mathbb{S}^d)}}. \tag{2.2}$$

We shall show that the right-hand side can be lower bounded in terms of ρ.

For the precise definition of f_ρ, we appeal to results of Hesse [12] by starting with the symmetric $C^\infty(\mathbb{R})$ function with support $[-1, 1]$,

$$\Phi(t) := \begin{cases} \exp\left(1 - \dfrac{1}{1 - t^2}\right) & \text{if } -1 < t < 1, \\ 0 & \text{otherwise.} \end{cases} \tag{2.3}$$

We rescale this function to have new support $[\cos\rho, \cos(\rho/2)]$ using the linear bijection g_ρ that maps this interval onto $[-1, 1]$ giving $\Phi_\rho(t) := \Phi(g_\rho(t))$ and then lift it to the sphere to get the zonal function

$$f_\rho(\mathbf{x}) := \Phi_\rho(\mathbf{y}_0 \cdot \mathbf{x}) = \Phi(g_\rho(\mathbf{y}_0 \cdot \mathbf{x})), \qquad \mathbf{x}, \mathbf{y}_0 \in \mathbb{S}^d. \tag{2.4}$$

The point $\mathbf{y}_0$ is chosen to be the center of a largest hole and thus achieves the maximum in (1.2). It is easily seen that $f_\rho \in C^\infty(\mathbb{S}^d)$ and that $f_\rho(\mathbf{x})$ vanishes unless $\cos(\rho/2) \geq \mathbf{y}_0 \cdot \mathbf{x} \geq \cos\rho$, so that the support of f_ρ is a collar within the spherical cap

$$S(\mathbf{y}_0; \rho) := \{\mathbf{x} \in \mathbb{S}^d : \mathbf{y}_0 \cdot \mathbf{x} \geq \cos\rho\}.$$

We now estimate the quantities on the right-hand side of (2.2). For $\mathrm{I}(f_\rho)$, the Funk–Hecke formula and a change of variable gives (also cf. [12, Eq. (32)])

$$|\mathrm{I}(f_\rho)| = \int_{\mathbb{S}^d} f_\rho(\mathbf{x}) \, d\sigma_d(\mathbf{x}) = \frac{\omega_{d-1}}{\omega_d} \int_{\rho/2}^{\rho} \Phi(g_\rho(\cos\theta)) (\sin\theta)^{d-1} \, d\theta \geq c_d \, \rho^d, \tag{2.5}$$

where ω_d is the surface area of $\mathbb{S}^d$. The Sobolev norm of f_ρ, computed as $\|f_\rho\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = \|(1 - \Delta_d^*)^{s/2} f_\rho\|_p$, is first estimated for even s. The result for other s is then obtained from the even case using Lemma 2.1. Let s be a non-negative even integer. Since f_ρ is zonal, use of spherical cylinder coordinates (cf. [18]) gives for $d \geq 1$:

$$(1 - \Delta_d^*)^{s/2} f_\rho(\mathbf{x}) = \left(1 + d \, t \, \mathrm{D}_t - (1 - t^2) \, \mathrm{D}_t^2\right)^{s/2} \Phi_\rho(t), \quad t = \mathbf{y}_0 \cdot \mathbf{x}, \tag{2.6}$$

where $\mathrm{D}_t := d/dt$. Expansion of the differential operator and term-wise estimation gives

$$\left|(1 - \Delta_d^*)^{s/2} f_\rho(\mathbf{x})\right| \leq c_{s,d} \left(\cos\frac{\rho}{2} - \cos\rho\right)^{-s/2} \leq c'_{s,d} \, \rho^{-s}, \qquad \mathbf{x} \in \mathbb{S}^d.$$

The details involve a slight modification of the arguments in [12], where a different constant is used in the differential operator $(1 - \Delta_d^*)^{s/2}$. The computations can also then be extended to include $d = 1$, a case not considered in [12]. Thus for $p = \infty$,

$$\|f_\rho\|_{\mathbb{W}_\infty^s(\mathbb{S}^d)} = \sup_{\mathbf{x} \in \mathbb{S}^d} \left|(1 - \Delta_d^*)^{s/2} f_\rho(\mathbf{x})\right| \leq c'_{s,d} \, \rho^{-s},$$

while for $1 \leq p < \infty$, since f_ρ is supported in $S(\mathbf{y}_0; \rho)$,

$$\|f_\rho\|_{\mathbb{W}_p^s(\mathbb{S}^d)}^p = \int_{\mathbb{S}^d} \left| (1 - \Delta_d^*)^{s/2} f_\rho(\mathbf{x}) \right|^p \mathrm{d}\sigma_d(\mathbf{x}) \leq (c'_{s,d})^p \, \rho^{-p\,s} \, \sigma_d(S(\mathbf{y}_0; \rho)) \leq (c''_{s,d})^p \, \rho^{-p\,s+d}.$$

Hence

$$\|f_\rho\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \leq c'''_{s,d} \, \rho^{-s+d/p}, \qquad 1 \leq p \leq \infty, \ s \geq 0 \text{ even}. \tag{2.7}$$

For general s, write $s = 2L + 2\theta$ with $0 \leq \theta \leq 1$ and L a non-negative integer. Then we can apply the interpolation inequality (2.1) with $s_0 = 2L$ and $s_1 = 2L + 2$ to obtain again

$$\|f_\rho\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \leq c_{s,d}^{iv} \, \rho^{-s+d/p}, \qquad 1 \leq p \leq \infty, \ s \geq 0. \tag{2.8}$$

Finally, using the estimates (2.5) and (2.8) in (2.2), we get

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \geq c_{s,d}^v \, \rho^{s+d/q},$$

where $1 \leq q \leq \infty$ is such that $1/p + 1/q = 1$. The proof is now complete. $\quad\square$

2.2. A generalization of the upper bound

We now provide a generalization of Theorem 1.2. Another way of describing the covering radius $\rho(X_N)$ is as the largest hole radius – more precisely, as the geodesic radius of the largest open spherical cap on $\mathbb{S}^d$ that does not contain a point of X_N. A (spherical cap shaped) hole of X_N can be any open spherical cap on $\mathbb{S}^d$ that does not contain points of X_N. Of particular interest are maximal holes, which are ones that lie "above" the facets of the convex hull of X_N. They are said to be maximal as they cannot be enlarged. Indeed, the supporting plane of a facet divides the sphere into an open spherical cap that contains no points of X_N and a closed one that contains all the points of X_N. These maximal holes provide a natural covering of the sphere with, in general, differently sized spherical caps of maximal radii. Among these maximal holes one can select a sequence of pairwise disjoint holes ordered with respect to non-increasing radii. This is a particular example of what we will call an "ordered X_N-avoiding packing on $\mathbb{S}^d$."

Definition 2.2. Given an N-point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ on $\mathbb{S}^d$, a sequence $(s_n)_{n \geq 1}$ of open pairwise disjoint spherical caps with cap radii $\rho_1 \geq \rho_2 \geq \rho_3 \geq \cdots$ such that no s_n contains points of X_N is called an *ordered X_N-avoiding packing on $\mathbb{S}^d$*.

The next theorem gives an upper bound of the nth-largest spherical cap radius in an ordered X_N-avoiding packing of $\mathbb{S}^d$.

Theorem 2.3. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ such that $1/p + 1/q = 1$ and $s > d/p$. Given an N-point set X_N on $\mathbb{S}^d$ and an ordered X_N-avoiding packing on $\mathbb{S}^d$ with spherical cap radii $\rho_1 \geq \rho_2 \geq \rho_3 \geq \cdots$, then*

$$\rho_n \leq c_{s,d} \, n^{-1/(qs+d)} \left[\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \right]^{1/(s+d/q)},$$

where the constant $c_{s,d}$ depends on s and d but not on p or q or the packing.

Proof. We proceed along the same lines as the proof of Theorem 1.2 but use now a fooling function of the form

$$F_n(\mathbf{x}) := \sum_{k=1}^n f_{\rho_k}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{S}^d,$$

that is the sum of all the contributions of functions $f_{\rho_k}(\mathbf{x}) := \Phi_{\rho_k}(\mathbf{y}_k \cdot \mathbf{x})$ of type (2.4) fitted to holes centered at $\mathbf{y}_k \in \mathbb{S}^d$, $1 \le k \le n$, in the ordered X_N-avoiding packing on $\mathbb{S}^d$.

From (2.5) we obtain that

$$|\mathrm{I}(F_n)| = \sum_{k=1}^{n} |\mathrm{I}(f_{\rho_k})| \ge c_d \sum_{k=1}^{n} \rho_k^d \ge n\, c_d\, \rho_n^d. \tag{2.9}$$

Observe that the supports of any two of $f_{\rho_1}, \ldots, f_{\rho_n}$ intersect at most on their boundaries. It follows that for even $s \ge 0$ this property also holds for any two of $\mathbf{J}_{-s}[f_{\rho_1}], \ldots, \mathbf{J}_{-s}[f_{\rho_n}]$, where $\mathbf{J}_{-s}[f_\rho] = (1 - \Delta_d^*)^{s/2} f_\rho$ (see (2.6)). The estimate (2.7) gives for $p = \infty$,

$$\|F_n\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = \max_{1 \le m \le n} \|f_{\rho_m}\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \le \max_{1 \le m \le n} c_{s,d}''' \rho_m^{-s} = c_{s,d}''' \rho_n^{-s},$$

while for $1 \le p < \infty$,

$$\|F_n\|_{\mathbb{W}_p^s(\mathbb{S}^d)}^p = \sum_{m=1}^{n} \|f_{\rho_m}\|_{\mathbb{W}_p^s(\mathbb{S}^d)}^p \le \sum_{m=1}^{n} \left(c_{s,d}''' \rho_m^{-s+d/p} \right)^p \le n \left(c_{s,d}''' \rho_n^{-s+d/p} \right)^p.$$

Hence

$$\|F_n\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \le n^{1/p}\, c_{s,d}'''\, \rho^{-s+d/p}, \qquad 1 \le p \le \infty,\ s \ge 0 \text{ even}. \tag{2.10}$$

The result for other s is then obtained using the interpolation inequality (2.1):

$$\|F_n\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \le n^{1/p}\, c_{s,d}^{iv}\, \rho^{-s+d/p}, \qquad 1 \le p \le \infty,\ s \ge 0 \text{ not even}. \tag{2.11}$$

Substituting the estimates (2.9), (2.10) and (2.11) into (2.2), we get

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \ge n^{1/q}\, c_{s,d}^v\, \rho_n^{s+d/q},$$

where $1 \le q \le \infty$ is such that $1/p + 1/q = 1$. This completes the proof. $\square$

2.3. Lower bound

Proof of Theorem 1.9. Let (Z_{N_t}) be a sequence of well-separated spherical t-designs on $\mathbb{S}^d$ with $N_t \asymp t^d$. The existence of such a sequence is established in [5]. Fix $\varepsilon \in (0, 1]$ and $c > 0$. For each Z_{N_t} we select a spherical cap with radius $\alpha_t = c\, N_t^{-(1-\varepsilon)/d}$ and an arbitrary center, and remove all the points in this cap. This gives a new set $X_{N_t - M_t}$ with $N_t - M_t$ points, where M_t depends on the cap and on α_t and thus on N_t. It follows from the well-separation property of (Z_{N_t}) that $\delta(X_{N_t - M_t}) \ge c' N_t^{-1/d}$ for some $c' > 0$, thus for some $c'' > 0$, we have

$$M_t \le c''\, N_t^\varepsilon \qquad \text{for all } Z_{N_t}.$$

The removal of the M_t points generates a hole of radius α_t, so that the covering radius of $X_{N_t - M_t}$ satisfies

$$\rho(X_{N_t - M_t}) \ge \alpha_t = c\, N_t^{-(1-\varepsilon)/d}. \tag{2.12}$$

Next, we quantify the quality of $X_{N_t - M_t}$ as a set of cubature points by estimating the worst-case error for the QMC method $\mathrm{Q}[X_{N_t - M_t}]$. Let $f \in \mathbb{W}_p^s(\mathbb{S}^d)$, $s > d/p$, with $\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = 1$. The error of numerical integration, $\mathcal{R}[X_{N_t - M_t}](f) := \mathrm{Q}[X_{N_t - M_t}](f) - \mathrm{I}[X_{N_t - M_t}](f)$, can be written as

$$\mathcal{R}[X_{N_t - M_t}](f) = \frac{N_t}{N_t - M_t} \mathcal{R}[Z_{N_t}](f) - \frac{M_t}{N_t - M_t} \mathcal{R}[Z_{N_t} \setminus X_{N_t - M_t}](f).$$

Since (Z_{N_t}) is a sequence of spherical t-designs with $N_t \asymp t^d$ and $N_t/(N_t - M) \to 1$ as $N_t \to \infty$, it follows from Proposition 1.3 that for some $C > 0$ we have

$$\frac{N_t}{N_t - M_t} |\mathcal{R}[Z_{N_t}](f)| \leq C\, N_t^{-s/d}.$$

Furthermore, the fact that $\mathbb{W}_p^s(\mathbb{S}^d)$ can be continuously embedded into $C(\mathbb{S}^d)$ for $s > d/p$ (Proposition 3.6) gives that for some $c_{p,s,d} > 0$ (embedding constant)

$$|\mathcal{R}[Z_{N_t} \setminus X_{N_t - M_t}](f)| \leq 2 \sup_{\mathbf{x} \in \mathbb{S}^d} |f(\mathbf{x})| \leq 2\, c_{p,s,d} \, \|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = 2\, c_{p,s,d}.$$

Since $M_t/(N_t - M_t) = \mathcal{O}(N_t^{-(1-\varepsilon)})$, we get

$$\frac{M_t}{N_t - M_t} |\mathcal{R}[Z_{N_t} \setminus X_{N_t - M_t}](f)| \leq 2\, c_{p,s,d} \frac{M_t}{N_t - M_t} \leq C'\, N_t^{-(1-\varepsilon)}.$$

We conclude that

$$\text{wce}(\text{Q}[X_{N_t - M_t}]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq C\, N_t^{-s/d} + C'\, N_t^{-(1-\varepsilon)}. \tag{2.13}$$

Until now we have allowed $\varepsilon \in (0, 1]$ to be arbitrary. If we now force $\varepsilon := 1 - s/d$, then $(X_{N_t - M_t})$ is a well-separated QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$. From (2.12) we have $\rho(X_{N_t - M_t}) \geq c\, N_t^{-s/d^2}$, completing the proof. $\square$

A more precise analysis of the effects on the worst-case error when one or more points are removed from a circular design (i.e., a spherical design on $\mathbb{S}^1$) is given in Section 7.

3. The function space setting and embedding theorems

In this section we set up the machinery needed to prove the worst-case error results. Let d be a positive integer. Our manifold is the unit sphere $\mathbb{S}^d$ in the Euclidean space $\mathbb{R}^{d+1}$ provided with the normalized surface area measure σ_d. For future reference we record that

$$\frac{\omega_{d-1}}{\omega_d} = \frac{\Gamma((d+1)/2)}{\sqrt{\pi}\,\Gamma(d/2)}, \qquad 2^{d-1} \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} (1 - t^2)^{d/2 - 1} \, \mathrm{d}t = 1, \tag{3.1}$$

where $\Gamma(z)$ denotes the gamma function, and ω_d is the surface area of $\mathbb{S}^d$.

3.1. Spherical harmonics

The restriction to $\mathbb{S}^d$ of a homogeneous and harmonic polynomial of total degree ℓ defined on $\mathbb{R}^{d+1}$ is called a *spherical harmonic* of degree ℓ on $\mathbb{S}^d$. The family $\mathcal{H}_\ell^d = \mathcal{H}_\ell^d(\mathbb{S}^d)$ of all spherical harmonics of exact degree ℓ on $\mathbb{S}^d$ has dimension

$$Z(d, \ell) := (2\ell + d - 1) \frac{\Gamma(\ell + d - 1)}{\Gamma(d)\Gamma(\ell + 1)}.$$

Each spherical harmonic Y_ℓ of exact degree ℓ is an eigenfunction of the negative *Laplace–Beltrami operator* $-\Delta_d^*$ for $\mathbb{S}^d$, with eigenvalue

$$\lambda_\ell := \ell\,(\ell + d - 1)\,, \qquad \ell = 0, 1, 2, \ldots. \tag{3.2}$$

As usual, let $\{Y_{\ell,k} : k = 1, \ldots, Z(d,\ell)\}$ denote an $\mathbb{L}_2$-orthonormal basis of $\mathcal{H}_\ell^d$. Then the basis functions $Y_{\ell,k}$ satisfy the following identity known as the *addition theorem*:

$$\sum_{k=1}^{Z(d,\ell)} Y_{\ell,k}(\mathbf{x})Y_{\ell,k}(\mathbf{y}) = Z(d,\ell)\,P_\ell^{(d)}(\mathbf{x} \cdot \mathbf{y}), \qquad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d, \tag{3.3}$$

where $P_\ell^{(d)}$ is the normalized Gegenbauer (or Legendre) polynomial, orthogonal on the interval $[-1, 1]$ with respect to the weight function $(1 - t^2)^{d/2-1}$, and normalized by $P_\ell^{(d)}(1) = 1$.

The collection $\{Y_{\ell,k} : k = 1, \ldots, Z(d,\ell); \ell = 0, 1, \ldots\}$ forms a complete orthonormal (with respect to σ_d) system for the Hilbert space $\mathbb{L}_2(\mathbb{S}^d)$ of square-integrable functions on $\mathbb{S}^d$ endowed with the usual inner product

$$(f, g)_{\mathbb{L}_2(\mathbb{S}^d)} := \int_{\mathbb{S}^d} f(\mathbf{x})g(\mathbf{x})\mathrm{d}\sigma_d(\mathbf{x}),$$

as well as a complete system for all the Banach spaces $\mathbb{L}_p(\mathbb{S}^d)$ of pth power integrable functions on $\mathbb{S}^d$ with $1 \le p < \infty$ provided with the usual p-norm

$$\|f\|_p := \|f\|_{\mathbb{L}_p(\mathbb{S}^d)} := \left(\int_{\mathbb{S}^d} |f(\mathbf{x})|^p \, \mathrm{d}\sigma_d(\mathbf{x}) \right)^{1/p},$$

and for the Banach space $C(\mathbb{S}^d)$ of continuous functions on $\mathbb{S}^d$ endowed with the maximum norm

$$\|f\|_C := \max_{\mathbf{x} \in \mathbb{S}^d} |f(\mathbf{x})|\,.$$

(For more details, we refer the reader to [2,18].)

The Funk–Hecke formula states that for every spherical harmonic Y_ℓ of degree ℓ (see [18]),

$$\int_{\mathbb{S}^d} g(\mathbf{y} \cdot \mathbf{z})\, Y_\ell(\mathbf{y})\, \mathrm{d}\sigma_d(\mathbf{y}) = \widehat{g}(\ell)\, Y_\ell(\mathbf{z}), \qquad \mathbf{z} \in \mathbb{S}^d, \tag{3.4}$$

where

$$\widehat{g}(\ell) = \frac{\omega_{d-1}}{\omega_d} \int_{-1}^1 g(t)\, P_\ell^{(d)}(t)\, \left(1 - t^2\right)^{d/2-1} \mathrm{d}t. \tag{3.5}$$

(This formula holds, in particular, for the spherical harmonic $Y_\ell(\mathbf{y}) = P_\ell^{(d)}(\mathbf{a} \cdot \mathbf{y})$, $\mathbf{a} \in \mathbb{S}^d$.)

3.2. Convolution

We shall frequently use the convolution of a zonal kernel, i.e. one that depends only on the inner product of the arguments, "against" a function f on $\mathbb{S}^d$. With abuse of notation we write $G(\mathbf{x}, \mathbf{y}) = G(\mathbf{x} \cdot \mathbf{y})$ for

$\mathbf{x}, \mathbf{y} \in \mathbb{S}^d$. For $1 \leq p < \infty$, let $\mathbb{L}_{p,d}([-1,1])$ consists of all functions of the form $g_{\mathbf{z}}(\mathbf{x}) := G(\mathbf{z} \cdot \mathbf{x})$, $\mathbf{x}, \mathbf{z} \in \mathbb{S}^d$, with finite norm $\|G\|_{p,d} := \|g_{\mathbf{z}}\|_p$. Of course, this norm does not depend on the choice of $\mathbf{z} \in \mathbb{S}^d$ since, by the Funk–Hecke formula with $\ell = 0$ (see (3.4) and (3.5)),

$$\|G\|_{p,d} = \|g_{\mathbf{z}}\|_p = \left(\frac{\omega_{d-1}}{\omega_d} \int\limits_{-1}^{1} |G(t)|^p \left(1 - t^2\right)^{d/2-1} \mathrm{d}t \right)^{1/p}. \tag{3.6}$$

Definition 3.1. The convolution of the zonal kernel $G \in \mathbb{L}_{1,d}([-1,1])$ against $f \in \mathbb{L}_p(\mathbb{S}^d)$ is the function $G * f$ given by

$$(G * f)(\mathbf{x}) := \int\limits_{\mathbb{S}^d} G(\mathbf{z} \cdot \mathbf{x}) f(\mathbf{z}) \, \mathrm{d}\sigma_d(\mathbf{z}), \qquad \mathbf{x} \in \mathbb{S}^d.$$

The convolution of the zonal kernel $K \in \mathbb{L}_{1,d}([-1,1])$ against $G \in \mathbb{L}_{1,d}([-1,1])$ is the kernel $K * G$ given by

$$(K * G)(\mathbf{x} \cdot \mathbf{y}) := \int\limits_{\mathbb{S}^d} K(\mathbf{z} \cdot \mathbf{x}) G(\mathbf{z} \cdot \mathbf{y}) \, \mathrm{d}\sigma_d(\mathbf{z}), \qquad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d.$$

If $g \in \mathbb{L}_{q,d}([-1,1])$, $1 \leq p, q \leq \infty$ and $f \in \mathbb{L}_p(\mathbb{S}^d)$, then the convolution $g * f$ exists σ_d-almost everywhere on $\mathbb{S}^d$ and Young's inequality holds; i.e.,

$$\|g * f\|_r \leq \|g\|_{q,d} \|f\|_p \qquad \text{for all } r \text{ with } \frac{1}{r} = \frac{1}{p} + \frac{1}{q} - 1 \geq 0. \tag{3.7}$$

In particular, one has

$$\|g * f\|_p \leq \|g\|_{1,d} \|f\|_p \qquad \text{and} \qquad \|g * f\|_q \leq \|g\|_{q,d} \|f\|_1. \tag{3.8}$$

3.3. Sobolev function space classes

The *Laplace–Fourier series* (in terms of spherical harmonics) of a function $f \in \mathbb{L}_1(\mathbb{S}^d)$ is given by the formal expansion

$$S[f](\mathbf{x}) \sim \sum_{\ell=0}^{\infty} Y_\ell[f](\mathbf{x}), \qquad \mathbf{x} \in \mathbb{S}^d, \tag{3.9}$$

where $Y_\ell[f]$ is the *projection of f onto $\mathcal{H}_\ell^d$*. It can be obtained by the convolution

$$Y_\ell[f](\mathbf{x}) := \int\limits_{\mathbb{S}^d} Z(d, \ell) P_\ell^{(d)}(\mathbf{x} \cdot \mathbf{y}) f(\mathbf{y}) \, \mathrm{d}\sigma_d(\mathbf{y}), \qquad \mathbf{x} \in \mathbb{S}^d. \tag{3.10}$$

Application of the addition theorem yields

$$Y_\ell[f](\mathbf{x}) = \sum_{k=1}^{Z(d,\ell)} \widehat{f}_{\ell,k} Y_{\ell,k}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{S}^d, \tag{3.11}$$

and $\widehat{f}_{\ell,k}$ are the *Laplace–Fourier coefficients* of f defined by

$$\widehat{f}_{\ell,k} := \int\limits_{\mathbb{S}^d} f(\mathbf{x}) Y_{\ell,k}(\mathbf{x}) \mathrm{d}\sigma_d(\mathbf{x}), \qquad k = 1, \ldots, Z(d, \ell), \ \ell = 0, 1, 2, \ldots. \tag{3.12}$$

Definition 3.2. The generalized Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ may be defined for $s \geq 0$ and $1 \leq p \leq \infty$ as the set of all functions $f \in \mathbb{L}_p(\mathbb{S}^d)$ with

$$\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} := \left\| \sum_{\ell=0}^{\infty} (1 + \lambda_\ell)^{s/2} Y_\ell[f] \right\|_p < \infty, \tag{3.13}$$

where the λ_ℓ are given in (3.2) and formulas for $Y_\ell[f]$ are provided in (3.10) and (3.11).

Remark. The definition implies that $\sum_{\ell=0}^{L} (1 + \lambda_\ell)^{s/2} Y_\ell[f](\mathbf{x})$ converges pointwise as $L \to \infty$ for almost all (in the sense of Lebesgue measure) points on $\mathbb{S}^d$, since otherwise the sum is not in $\mathbb{L}_p(\mathbb{S}^d)$.

We note that $\mathbb{W}_p^0(\mathbb{S}^d) = \mathbb{L}_p(\mathbb{S}^d)$. In the case of $p = 2$, Parseval's identity yields the following equivalent characterization: a function $f \in \mathbb{L}_2(\mathbb{S}^d)$ is in $\mathbb{W}_2^s(\mathbb{S}^d)$ if and only if the Laplace–Fourier coefficients $\widehat{f}_{\ell,k}$ of f given in (3.12) satisfy the condition

$$\sum_{\ell=0}^{\infty} (1 + \lambda_\ell)^s \sum_{k=1}^{Z(d,\ell)} \left| \widehat{f}_{\ell,k} \right|^2 < \infty, \tag{3.14}$$

but a characterization of this kind in terms of the Laplace–Fourier coefficients does not hold for general p.

3.4. The space $\mathbb{W}_p^s(\mathbb{S}^d)$ as a Bessel potential space

The *Bessel operator of order s*,

$$\mathbf{J}_{-s} := (1 - \Delta_d^*)^{s/2}, \qquad s \in \mathbb{R}, \tag{3.15}$$

is a pseudodifferential operator of order s with symbol $(b_\ell^{(s)})_{\ell \geq 0}$ given by

$$b_\ell^{(s)} := (1 + \lambda_\ell)^{s/2} \asymp (1 + \ell)^s, \qquad \ell = 0, 1, 2, \ldots. \tag{3.16}$$

For $s \geq 0$ it is an operator from $\mathbb{W}_p^s(\mathbb{S}^d)$ to $\mathbb{L}_p(\mathbb{S}^d)$ defined by

$$\mathbf{J}_{-s}[f] := \sum_{\ell=0}^{\infty} b_\ell^{(s)} Y_\ell[f]. \tag{3.17}$$

We shall also need the inverse operator $\mathbf{J}_s : \mathbb{L}_p(\mathbb{S}^d) \to \mathbb{W}_p^s(\mathbb{S}^d)$, which, in contrast to $\mathbf{J}_{-s}$ for $s \geq 0$, is a smoothing operator. The Bessel operator satisfies the following identities:

$$\mathbf{J}_{-\alpha} \mathbf{J}_{-\beta} = \mathbf{J}_{-(\alpha+\beta)}, \qquad (\mathbf{J}_{-\alpha})^{-1} = \mathbf{J}_\alpha, \qquad \mathbf{J}_0 = \mathrm{Id}, \qquad \alpha, \beta \in \mathbb{R}. \tag{3.18}$$

The generalized Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ of Definition 3.2 can be interpreted as a *Bessel potential space* and we can use the following equivalent characterization.

Proposition 3.3. *Let $s \geq 0$ and $1 \leq p \leq \infty$. Then $\mathbb{W}_p^s(\mathbb{S}^d)$ is the set of all functions $f \in \mathbb{L}_p(\mathbb{S}^d)$ for which $\mathbf{J}_{-s}[f] \in \mathbb{L}_p(\mathbb{S}^d)$, and $\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = \|\mathbf{J}_{-s}[f]\|_p$.*

For $s \geq 0$ we define the zonal *Bessel kernel*

$$B^{(s)}(\mathbf{x} \cdot \mathbf{y}) := \sum_{\ell=0}^{\infty} b_{\ell}^{(-s)} Z(d,\ell) P_{\ell}^{(d)}(\mathbf{x} \cdot \mathbf{y}), \qquad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d. \tag{3.19}$$

Then we can use the following characterization of $\mathbb{W}_p^s(\mathbb{S}^d)$.

Proposition 3.4. *Let $s \geq 0$ and $1 \leq p \leq \infty$. Then $f \in \mathbb{W}_p^s(\mathbb{S}^d)$ if and only if f is a Bessel potential of a function $g \in \mathbb{L}_p(\mathbb{S}^d)$; that is,*

$$f(\mathbf{x}) = \int_{\mathbb{S}^d} B^{(s)}(\mathbf{y} \cdot \mathbf{x}) \, g(\mathbf{y}) \, \mathrm{d}\sigma_d(\mathbf{y}) = \left(B^{(s)} * g\right)(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{S}^d. \tag{3.20}$$

Moreover, we have $\mathbf{J}_{-s}[f] = g$ and $\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = \|g\|_p$.

Indeed, any convolution (3.20) is in $\mathbb{W}_p^s(\mathbb{S}^d)$ by Young's inequality together with the following boundedness result. (The proof will be postponed until the end of Section 5.)

Lemma 3.5 *(Boundedness of the $\mathbb{L}_q(\mathbb{S}^d)$-norm of the Bessel kernel). Let $d \geq 1$, $1 \leq p, q \leq \infty$ such that $1/p + 1/q = 1$ and $s > d/p$. Then there exists a constant $c > 0$ such that*

$$\left\|B^{(s)}\right\|_{q,d} \leq 1 + \frac{c}{1 - 2^{d/p-s}}. \tag{3.21}$$

We remark that for $p = 2$, the generalized Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ is a reproducing kernel Hilbert space with reproducing kernel $B^{(2s)}$ (cf. [9, Sec. 2.4]). For further reading on Bessel potential spaces, we refer to the classical paper [29] and the more recent paper [15]. For the spherical case, we rely on [6].

3.5. Embedding results

For the reader's convenience, we briefly summarize some relevant embedding results (see, e.g., Aubin [1]).

Proposition 3.6 *(Continuous embedding into $C(\mathbb{S}^d)$). Let $d \geq 1$. The Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ is continuously embedded into $C(\mathbb{S}^d)$ if $s > d/p$.*

For fixed p, smoother Sobolev spaces are included in coarser ones:

Proposition 3.7 *(Continuous embedding, p fixed). Let $d \geq 1$. For fixed p with $1 \leq p \leq \infty$, $\mathbb{W}_p^{s'}(\mathbb{S}^d)$ is continuously embedded into $\mathbb{W}_p^s(\mathbb{S}^d)$ if $0 \leq s < s' < \infty$.*

The standard embedding results for $\mathbb{L}_p$-spaces immediately yield the following embedding of $\mathbb{W}_{p'}^s(\mathbb{S}^d)$ into $\mathbb{W}_p^s(\mathbb{S}^d)$, $p < p'$:

Proposition 3.8 *(Continuous embedding, s fixed). Let $d \geq 1$. For fixed s with $0 \leq s < \infty$, $\mathbb{W}_{p'}^s(\mathbb{S}^d)$ is continuously embedded into $\mathbb{W}_p^s(\mathbb{S}^d)$ if $1 \leq p < p' \leq \infty$.*

4. Worst-case error and QMC-design sequences for $\mathbb{W}_p^s(\mathbb{S}^d)$

4.1. Worst-case error

We recall that the definition of worst-case error is given in (1.4). Let $\nu_N := \nu[X_N]$ be the atomic measure associated with $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ that places the point mass $1/N$ at each point in X_N; i.e.,

$$\nu_N = \nu[X_N] = \frac{1}{N} \sum_{j=1}^{N} \delta_{\mathbf{x}_j}.$$

Then the error of integration of a continuous function f on $\mathbb{S}^d$ can be written as

$$Q[X_N](f) - I(f) = \int_{\mathbb{S}^d} f(\mathbf{x}) \, d\mu_N(\mathbf{x}),$$

with the signed measure μ_N defined by $\mu_N = \nu_N - \sigma_d$. For the Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ with $s > d/p$, the worst-case error has the following form in terms of the Bessel kernel: let

$$\mathcal{B}^{(s)}(t) := B^{(s)}(t) - 1 = \sum_{\ell=1}^{\infty} b_\ell^{(-s)} Z(d, \ell) P_\ell^{(d)}(t), \qquad -1 \leq t \leq 1, \tag{4.1}$$

then the worst-case error is equal to the $\mathbb{L}_q(\mathbb{S}^d)$-norm of the following function,

$$\mathcal{B}_N^{(s)}(\mathbf{y}) := \mathcal{B}^{(s)}[X_N](\mathbf{y}) := \frac{1}{N} \sum_{j=1}^{N} B^{(s)}(\mathbf{x}_j \cdot \mathbf{y}) - 1 = \frac{1}{N} \sum_{j=1}^{N} \mathcal{B}^{(s)}(\mathbf{x}_j \cdot \mathbf{y}), \qquad \mathbf{y} \in \mathbb{S}^d. \tag{4.2}$$

For each fixed $\mathbf{y} \in \mathbb{S}^d$, this function represents the error of numerical integration of the zonal function $\mathbf{x} \mapsto B^{(s)}(\mathbf{x} \cdot \mathbf{y})$, $\mathbf{x} \in \mathbb{S}^d$, of the QMC method based on the node set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$.

Theorem 4.1. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ and $s > d/p$. Then, for a QMC method $Q[X_N]$ with node set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$,*

$$\text{wce}(Q[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) = \left\| \int_{\mathbb{S}^d} B^{(s)}(\mathbf{x} \cdot \cdot) d\mu_N(\mathbf{x}) \right\|_q = \left\| \mathcal{B}_N^{(s)} \right\|_q. \tag{4.3}$$

Remark. In the Hilbert space setting $p = q = 2$, one has the closed form representation

$$\left\| \mathcal{B}_N^{(s)} \right\|_2 = \left(\frac{1}{N^2} \sum_{j=1}^{N} \sum_{k=1}^{N} \mathcal{B}^{(2s)}(\mathbf{x}_j \cdot \mathbf{x}_k) \right)^{1/2}, \tag{4.4}$$

which follows from the relation

$$\int_{\mathbb{S}^d} B^{(\alpha)}(\mathbf{x} \cdot \mathbf{z}) B^{(\beta)}(\mathbf{y} \cdot \mathbf{z}) \, d\sigma_d(\mathbf{z}) = B^{(\alpha+\beta)}(\mathbf{x} \cdot \mathbf{y}), \qquad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d, \ \alpha, \beta > 0. \tag{4.5}$$

Proof of Theorem 4.1. First, note that the last expression in (4.3) follows from substituting $\mu_N = \nu_N - \sigma_d$ into the middle expression in (4.3). Since $s > d/p$, the Sobolev space $\mathbb{W}_p^s(\mathbb{S}^d)$ is continuously embedded into $C(\mathbb{S}^d)$ by Proposition 3.6, and every element in $\mathbb{W}_p^s(\mathbb{S}^d)$ has a continuous representative. For $f \in \mathbb{W}_p^s(\mathbb{S}^d)$ the following inequality, due to [6, Corollary 2.4], can be derived from (3.20) together with Fubini's theorem and Hölder's inequality,

$$\left| \int_{\mathbb{S}^d} f(\mathbf{x}) \mathrm{d}\mu_N(\mathbf{x}) \right| \leq \left\{ \int_{\mathbb{S}^d} \left| \int_{\mathbb{S}^d} B^{(s)}(\mathbf{x} \cdot \mathbf{y}) \mathrm{d}\mu_N(\mathbf{x}) \right|^q \mathrm{d}\sigma_d(\mathbf{y}) \right\}^{1/q} \|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)}. \tag{4.6}$$

These integrals are well defined and finite. Therefore,

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq \left\| \int_{\mathbb{S}^d} B^{(s)}(\mathbf{x} \cdot \cdot) \mathrm{d}\mu_N(\mathbf{x}) \right\|_q = \left\| \mathcal{B}_N^{(s)} \right\|_q. \tag{4.7}$$

We complete the proof by constructing a bad function $f_{\mathbf{bad}}$ with $\|f_{\mathbf{bad}}\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = 1$ whose absolute integration error is equal to the right-hand side above when $1 \leq q < \infty$, and giving a lower estimate argument for $\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d))$ in the case $q = \infty$. Let $1 \leq q < \infty$ and $1/p + 1/q = 1$. Consider the function $\mathcal{B}_N^{(s)}$ from (4.2). As $\mathcal{B}_N^{(s)} \in \mathbb{L}_q(\mathbb{S}^d)$, there exists a function $u \in \mathbb{L}_p(\mathbb{S}^d)$ such that

$$\|u\|_p = 1 \qquad \text{and} \qquad \left| \int_{\mathbb{S}^d} \mathcal{B}_N^{(s)}(\mathbf{y}) u(\mathbf{y}) \mathrm{d}\sigma_d(\mathbf{y}) \right| = \left\| \mathcal{B}_N^{(s)} \right\|_q:$$

one can choose

$$u(\mathbf{y}) = \begin{cases} \dfrac{\left| \mathcal{B}_N^{(s)}(\mathbf{y}) \right|^{q-1}}{\left\| \mathcal{B}_N^{(s)} \right\|_q^{q-1}} \dfrac{\left| \mathcal{B}_N^{(s)}(\mathbf{y}) \right|}{\mathcal{B}_N^{(s)}(\mathbf{y})} & \text{if } \mathcal{B}_N^{(s)}(\mathbf{y}) \neq 0, \\ 0 & \text{if } \mathcal{B}_N^{(s)}(\mathbf{y}) = 0, \end{cases} \qquad \mathbf{y} \in \mathbb{S}^d.$$

Now, set $v = \mathbf{J}_s[u]$. Then $v \in \mathbb{W}_p^s(\mathbb{S}^d)$. In fact, by definition of u,

$$\|v\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = \|\mathbf{J}_{-s}[v]\|_p = \|\mathbf{J}_{-s}[\mathbf{J}_s[u]]\|_p = \|u\|_p = 1.$$

The bad function $f_{\mathbf{bad}}$ with $\|f_{\mathbf{bad}}\|_{\mathbb{W}_p^s(\mathbb{S}^d)} = 1$ is now the continuous representative of v in $\mathbb{W}_p^s(\mathbb{S}^d)$. Because of the convolution formula $\mathbf{J}_s[u] = B^{(s)} * u$, we obtain for the absolute error of numerical integration by the QMC method $\mathrm{Q}[X_N]$,

$$\left| \int_{\mathbb{S}^d} f_{\mathbf{bad}}(\mathbf{x}) \, \mathrm{d}\mu_N(\mathbf{x}) \right| = \left| \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} B^{(s)}(\mathbf{x} \cdot \mathbf{y}) u(\mathbf{y}) \, \mathrm{d}\sigma_d(\mathbf{y}) \mathrm{d}\mu_N(\mathbf{x}) \right|$$

$$= \left| \int_{\mathbb{S}^d} u(\mathbf{y}) \mathcal{B}_N^{(s)}(\mathbf{y}) \, \mathrm{d}\sigma_d(\mathbf{y}) \right| = \left\| \mathcal{B}_N^{(s)} \right\|_q.$$

This lower bound of $\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d))$ matches the upper bound in (4.7).

Let $q = \infty$ (i.e., $p = 1$). By the definition of the $\mathbb{L}_\infty(\mathbb{S}^d)$-norm, to every $\varepsilon > 0$ there exists a subset $E_\varepsilon \subset \mathbb{S}^d$ of positive σ_d-measure such that $|\mathcal{B}_N^{(s)}(\mathbf{y})| \geq \|\mathcal{B}_N^{(s)}\|_\infty - \varepsilon$ on E_ε and a function $u_\varepsilon \in \mathbb{L}_1(\mathbb{S}^d)$ satisfying

$$\|u_\varepsilon\|_1 = 1 \qquad \text{and} \qquad \left| \int_{\mathbb{S}^d} \mathcal{B}_N^{(s)}(\mathbf{y}) \, u_\varepsilon(\mathbf{y}) \mathrm{d}\sigma_d(\mathbf{y}) \right| \geq \left\| \mathcal{B}_N^{(s)} \right\|_\infty - \varepsilon.$$

One can choose

$$u_\varepsilon(\mathbf{y}) = \begin{cases} \dfrac{\chi_\varepsilon(\mathbf{y})}{\sigma_d(E_\varepsilon)} \dfrac{\left| \mathcal{B}_N^{(s)}(\mathbf{y}) \right|}{\mathcal{B}_N^{(s)}(\mathbf{y})} & \text{if } \mathcal{B}_N^{(s)}(\mathbf{y}) \neq 0, \\ 0 & \text{if } \mathcal{B}_N^{(s)}(\mathbf{y}) = 0, \end{cases} \qquad \mathbf{y} \in \mathbb{S}^d,$$

where $\chi_\varepsilon := \chi_{E_\varepsilon}$ is the characteristic function of the set E_ε. Similarly as before, one shows that $v_\varepsilon = \mathbf{J}_s[u_\varepsilon]$ is in $\mathbb{W}_1^s(\mathbb{S}^d)$ and $\|v_\varepsilon\|_{\mathbb{W}_1^s(\mathbb{S}^d)} = 1$. Taking $f_{\mathbf{bad},\varepsilon}$ to be the continuous representative of v_ε in $\mathbb{W}_1^s(\mathbb{S}^d)$, we arrive at

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_1^s(\mathbb{S}^d)) \geq \left| \int_{\mathbb{S}^d} f_{\mathbf{bad},\varepsilon}(\mathbf{x}) \, \mathrm{d}\mu_N(\mathbf{x}) \right| = \left| \int_{\mathbb{S}^d} \mathcal{B}_N^{(s)}(\mathbf{y}) \, u_\varepsilon(\mathbf{y}) \mathrm{d}\sigma_d(\mathbf{y}) \right| \geq \left\| \mathcal{B}_N^{(s)} \right\|_\infty - \varepsilon.$$

Since $\varepsilon > 0$ is arbitrary, we have

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_1^s(\mathbb{S}^d)) \geq \left\| \mathcal{B}_N^{(s)} \right\|_\infty.$$

The result follows. $\quad\square$

4.2. WCE inequalities

The following property holds for the worst-case error of a QMC method for generalized Sobolev spaces with the same s but different p.

Theorem 4.2. *Let $d \geq 1$, $1 \leq p < p' \leq \infty$ and $s > d/p$. For every N-point set $X_N \subset \mathbb{S}^d$,*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_{p'}^s(\mathbb{S}^d)) \leq \mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)). \tag{4.8}$$

Proof. Let $1 \leq p < p' \leq \infty$ and $s > d/p$. Then one has the continuous embedding inclusions $\mathbb{W}_{p'}^s(\mathbb{S}^d) \subset \mathbb{W}_p^s(\mathbb{S}^d) \subset C(\mathbb{S}^d)$ and, in particular, $\|f\|_{\mathbb{W}_p^s(\mathbb{S}^d)} \leq c \|f\|_{\mathbb{W}_{p'}^s(\mathbb{S}^d)}$ with $c = 1$ because of $\int_{\mathbb{S}^d} \mathrm{d}\sigma_d = 1$ (Proposition 3.3 and Jensen's inequality). Thus, the unit ball in $\mathbb{W}_p^s(\mathbb{S}^d)$ is larger than the one in $\mathbb{W}_{p'}^s(\mathbb{S}^d)$ and the result follows from (1.4). $\quad\square$

As a consequence of Theorem 4.2 we provide the following proof.

Proof of Theorem 1.10. Let (X_N) be a QMC-design sequence for $\mathbb{W}_p^s(\mathbb{S}^d)$, where $1 \leq p < \infty$ and $s > d/p$. Then, there exists a constant $c > 0$ such that $\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq c N^{-s/d}$ for all X_N. Suppose $p < p' \leq \infty$. Then by Theorem 4.2,

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_{p'}^s(\mathbb{S}^d)) \leq \mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \leq c N^{-s/d} \qquad \text{for all } X_N.$$

Hence by Definition 1.4, (X_N) is a QMC-design sequence for $\mathbb{W}_{p'}^s(\mathbb{S}^d)$. $\quad\square$

Next, we consider worst-case error interrelations for generalized Sobolev spaces with the same p but different s. In the Hilbert space setting $p = 2$ the reproducing kernel Hilbert space method gives a heat kernel representation of the worst-case error which leads to the following result.

Proposition 4.3. *(See [9, Lemma 26].) Let $d \geq 1$ and $s > d/2$. If* $\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_2^s(\mathbb{S}^d)) < 1$*, then*

$$\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_2^{s'}(\mathbb{S}^d)) < c_{d,s,s'} \left[\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_2^s(\mathbb{S}^d)) \right]^{s'/s}, \qquad d/2 < s' < s, \tag{4.9}$$

where $c_{d,s,s'} > 0$ depends on the norms for $\mathbb{W}_2^s(\mathbb{S}^d)$ and $\mathbb{W}_2^{s'}(\mathbb{S}^d)$, but is independent of N.

The proof of Theorem 1.11 is based on the following $\mathbb{L}_q(\mathbb{S}^d)$-Bernstein type inequality.

Lemma 4.4. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ and $s - d/p > \tau > 0$. Then the function $\mathcal{B}_N^{(s)}$ for an N-point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$ with mesh ratio $\gamma(X_N)$ satisfies*

$$\left\| \mathcal{B}_N^{(s)} \right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \leq c \left[\gamma(X_N) \right]^{d/p} N^{\tau/d} \left\| \mathcal{B}_N^{(s)} \right\|_q, \tag{4.10}$$

where $c \geq 1$ depends only on d, p or q, s and τ.

We will provide a proof of (4.10) in Section 6.

Remark. Mhaskar et al. [17, Theorem 6.1, p. 1669] prove (4.10) for quasi-uniform X_N. Our estimate holds for general sequences (X_N) but is specific to the kernel $\mathcal{B}_N^{(s)}$. An essential feature of (4.10) is the explicit dependence on the mesh ratio of the point set. This is of importance for determining the stability and error estimates, and thus is of independent interest.

Proof of Theorem 1.11. First, we note that for fixed $\mathbf{x} \in \mathbb{S}^d$ the function $\phi^{(s')}(\mathbf{y}) := B^{(s')}(\mathbf{x} \cdot \mathbf{y})$, $\mathbf{y} \in \mathbb{S}^d$, is in $\mathbb{L}_q(\mathbb{S}^d)$ for $s' > d/p$ by Lemma 3.5. Then the identity (4.5) (with $\alpha = s'$ and $\beta = s - s'$) gives

$$\phi^{(s)}(\mathbf{y}) = \int_{\mathbb{S}^d} B^{(s-s')}(\mathbf{z} \cdot \mathbf{y}) \, \phi^{(s')}(\mathbf{z}) \, \mathrm{d}\sigma_d(\mathbf{z}), \qquad \mathbf{y} \in \mathbb{S}^d.$$

Consequently, $\mathcal{B}_N^{(s)}$ given in (4.2) is the Bessel potential of $\mathcal{B}_N^{(s')} \in \mathbb{L}_q(\mathbb{S}^d)$ in the sense of Proposition 3.4. Hence, by Theorem 4.1, Proposition 3.4 and Lemma 4.4 (with $\tau = s - s'$),

$$\begin{aligned}
\mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^{s'}(\mathbb{S}^d)) = \left\| \mathcal{B}_N^{(s')} \right\|_q &= \left\| \mathcal{B}_N^{(s)} \right\|_{\mathbb{W}_q^{s-s'}(\mathbb{S}^d)} \\
&\leq c \left[\gamma(X_N) \right]^{d/p} N^{(s-s')/d} \left\| \mathcal{B}_N^{(s)} \right\|_q \\
&= c \left[\gamma(X_N) \right]^{d/p} N^{(s-s')/d} \, \mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)), \tag{4.11}
\end{aligned}$$

where the constant c depends on d, s, s', p. This completes the proof. $\square$

5. Filtered Bessel kernel and proof of Lemma 3.5

In this section we use a filtered Bessel kernel to prove Lemma 3.5. Let $d \geq 1$, $s \in \mathbb{R}$. Given a filter h (i.e., a smooth function on $\mathbb{R}_+$ with compact support), we define the *filtered Bessel kernel*

$$B_h^{(s)}(T; \mathbf{x} \cdot \mathbf{y}) := \sum_{\ell=0}^{\infty} h\left(\frac{\ell}{T}\right) b_\ell^{(-s)} Z(d, \ell) P_\ell^{(d)}(\mathbf{x} \cdot \mathbf{y}), \qquad T \geq 1, \mathbf{x}, \mathbf{y} \in \mathbb{S}^d. \tag{5.1}$$

In the special case $s = 0$, so $b_\ell^{(-s)} = 1$, the following results are known from [20]. The more general filtered Bessel kernel in (5.1) satisfies the following localization estimate.

Proposition 5.1 *(Localized upper bound; cf. [6, Lemma 2.8]). Let h be a filter with support $[1/2, 2]$. For every positive integer n, there exists a constant $c_n > 0$ such that for every $T > 1$ and $s \geq 0$,*

$$\left| B_h^{(s)}(T; \mathbf{x} \cdot \mathbf{y}) \right| \leq c_n \frac{T^{d-s}}{\left(1 + T^2 \left| \mathbf{x} - \mathbf{y} \right|^2 \right)^{n/2}}, \qquad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d. \tag{5.2}$$

Note that the upper bound is a zonal function, since $|\mathbf{x} - \mathbf{y}|^2 = 2 - 2\mathbf{x} \cdot \mathbf{y}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{S}^d$. The localized upper bound gives the following estimate in which $s > d/p$ to ensure that we are dealing with continuous functions.

Lemma 5.2 *($\mathbb{L}_q(\mathbb{S}^d)$-norm of filtered Bessel kernel). Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ and $s > d/p$. Suppose h is a filter with support $[1/2, 2]$. Then there exists a constant $c > 0$ such that*

$$\left\| B_h^{(s)}(T; \cdot) \right\|_{q,d} \leq c\, T^{d/p-s}, \qquad T \geq 1. \tag{5.3}$$

The constant c depends only on h, d, s and q.

Proof. First, let $1 \leq q < \infty$. Then

$$\left\| B_h^{(s)}(T; \cdot) \right\|_{q,d}^q = \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} \left| B_h^{(s)}(T; t) \right|^q \left(1 - t^2 \right)^{d/2-1} \mathrm{d}t.$$

The change of variable $2u = 1 + t$ and the localized estimate (5.2) give

$$\left\| B_h^{(s)}(T; \cdot) \right\|_{q,d}^q \leq G(T) := 2^{d-1} \frac{\omega_{d-1}}{\omega_d} \int_0^1 \frac{c_n^q\, T^{q(d-s)}}{\left(1 + 4T^2 - 4T^2 u \right)^{qn/2}} u^{d/2-1} \left(1 - u \right)^{d/2-1} \mathrm{d}u$$

for $T > 1$ and positive integers n. Rewriting the integral as

$$G(T) = \left[\frac{c_n\, T^{d-s}}{\left(1 + 4T^2 \right)^{n/2}} \right]^q 2^{d-1} \frac{\omega_{d-1}}{\omega_d} \int_0^1 \frac{u^{d/2-1} \left(1 - u \right)^{d/2-1}}{\left(1 - \frac{4T^2}{1+4T^2} u \right)^{qn/2}} \mathrm{d}u,$$

we express $G(T)$ in terms of a Gauss hypergeometric function (cf. [22, Eq. 15.6.1])

$$G(T) = \left[\frac{c_n\, T^{d-s}}{\left(1 + 4T^2 \right)^{n/2}} \right]^q {}_2\mathrm{F}_1 \left(\begin{matrix} qn/2, d/2 \\ d \end{matrix}; \frac{4T^2}{1 + 4T^2} \right).$$

A linear transformation of hypergeometric functions [22, last of Eq. 15.8.1] yields

$$G(T) = \left[\frac{c_n\, T^{d-s}}{\left(1 + 4T^2 \right)^{n/2}} \right]^q \left(\frac{1}{1 + 4T^2} \right)^{d/2-qn/2} {}_2\mathrm{F}_1 \left(\begin{matrix} qn/2, d/2 \\ d \end{matrix}; \frac{4T^2}{1 + 4T^2} \right).$$

Now choose n to be a fixed integer satisfying $n > 2d/q$. Because $d - qn/2 < 0$, the hypergeometric function part is strictly monotonically decreasing on $[0, \infty)$ as a function of T. This can be seen from the integral

representation (cf. [22, Eq. 15.6.1]) of the hypergeometric function and the fact that $4T^2/(1+4T^2)$ is strictly increasing on $[0, \infty)$. Then

$$
{}_2F_1\left(\begin{matrix} qn/2, d/2 \\ d \end{matrix}; \frac{4T^2}{1+4T^2}\right) \leq {}_2F_1\left(\begin{matrix} qn/2, d/2 \\ d \end{matrix}; 0\right) = 1.
$$

We arrive at

$$
\left\|B_h^{(s)}(T; \cdot)\right\|_{q,d} \leq c_n \frac{T^{d-s}}{(1+4T^2)^{d/(2q)}} \leq \frac{c_n}{2^{d/q}} T^{d(1-1/q)-s} \qquad \text{for } T \geq 1.
$$

The result follows for $1 \leq q < \infty$.

Let $q = \infty$. Using the localized estimate (5.2), we get for any fixed positive integer n,

$$
\left\|B_h^{(s)}(T; \cdot)\right\|_{\infty,d} = \max_{-1 \leq t \leq 1}\left|B_h^{(s)}(T; t)\right| \leq \max_{-1 \leq t \leq 1} \frac{c_n\, T^{d-s}}{(1+2T^2-2T^2\, t)^{n/2}} = c_n\, T^{d-s}
$$

for $T \geq 1$. This completes the proof. $\square$

In order to show that the $\mathbb{L}_q(\mathbb{S}^d)$-norm of the zonal Bessel kernel is bounded, we now strengthen the requirement on the filter h with support $[1/2, 2]$ occurring in the filtered Bessel kernel (5.1), by assuming that

$$
h(2t) + h(t) = 1 \qquad \text{on } [1/2, 1]. \tag{5.4}
$$

This condition is equivalent to saying that h has the *partition of unity property* (see [19]), namely

$$
\sum_{m=0}^{\infty} h\left(\frac{x}{2^m}\right) = 1 \qquad \text{for all } x \geq 1. \tag{5.5}
$$

Proof of Lemma 3.5. Let h be a filter with support $[1/2, 2]$ and the partition of unity property. Then using (5.1) and (5.5), we get

$$
\sum_{m=1}^{\infty} B_h^{(s)}(2^{m-1}; t) = \sum_{\ell=1}^{\infty}\left(\sum_{m=1}^{\infty} h\left(\frac{\ell}{2^{m-1}}\right)\right) b_\ell^{(-s)}\, Z(d, \ell) P_\ell^{(d)}(t) = B^{(s)}(t) - 1, \quad -1 \leq t \leq 1.
$$

Then for $s > d/p$ the triangle inequality and the filtered Bessel kernel estimate (5.3) yield

$$
\left\|B^{(s)} - 1\right\|_{q,d} = \left\|\sum_{m=1}^{\infty} B_h^{(s)}(2^{m-1}; \cdot)\right\|_{q,d} \leq \sum_{m=0}^{\infty}\left\|B_h^{(s)}(2^m; \cdot)\right\|_{q,d} \leq c\sum_{m=0}^{\infty}(2^m)^{d/p-s} = \frac{c}{1-2^{d/p-s}},
$$

where c is the constant in Lemma 5.2. On observing that $\|1\|_{q,d} = 1$, we get

$$
\left\|B^{(s)}\right\|_{q,d} \leq \left\|B^{(s)} - 1\right\|_{q,d} + \|1\|_{q,d} \leq 1 + \frac{c}{1-2^{d/p-s}}.
$$

This completes the proof. $\square$

6. Proof of Lemma 4.4

In this section, we prove the Bernstein type inequality (4.10) for the function

$$\mathcal{B}_N^{(s)}(\mathbf{y}) = \frac{1}{N} \sum_{j=1}^{N} \mathcal{B}^{(s)}(\mathbf{x}_j \cdot \mathbf{y}), \qquad \mathbf{y} \in \mathbb{S}^d,$$

which is central to the computation of the worst-case error (see Theorem 4.1).

In order to establish this result, we make use of the well-known Bernstein inequality for spherical polynomials (see [16, Proposition 4.3] and [27, Theorem 2]).

Proposition 6.1. *For $d \geq 1$, $1 \leq q \leq \infty$ and $\tau \geq 0$, there holds*

$$\|P\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \leq c_{q,\tau,d}\, n^\tau \, \|P\|_q\,, \qquad P \in \Pi_n^d, \tag{6.1}$$

where Π_n^d denotes the family of spherical polynomials on $\mathbb{S}^d$ of degree at most n.

We follow the general approach of [17], but with the crucial difference that we are able to replace a positive-definite assumption in [17] by the precise lower bound

$$\left\|\mathcal{B}_N^{(s)}\right\|_q = \mathrm{wce}(\mathrm{Q}[X_N]; \mathbb{W}_p^s(\mathbb{S}^d)) \geq \frac{c'_{p,s,d}}{N^{s/d}} > 0, \qquad s > \frac{d}{p}, \quad \frac{1}{p} + \frac{1}{q} = 1, \tag{6.2}$$

which follows from Theorem 4.1 and the lower bound of Proposition 1.6. Our strategy is to approximate $\mathcal{B}_N^{(s)}$ by spherical polynomials on $\mathbb{S}^d$ of degree $2^m \asymp N^{1/d}$ that are convolution approximations of $\mathcal{B}_N^{(s)}$ with filtered Bessel kernels. For a smooth filter $\widetilde{h}$ with support $[0, 2]$, to be specified below, we define (see (5.1) and (3.16))

$$\eta_0 \equiv 1, \qquad \eta_m := \eta_{m,\widetilde{h}} := B_{\widetilde{h}}^{(0)}(2^{m-1}; \cdot), \quad m \geq 1.$$

Then it can be readily seen that $\eta_m * \mathcal{B}_N^{(s)}$ is a spherical polynomial of degree $2^m - 1$. By (4.5), $\mathcal{B}_N^{(s)}$ is the Bessel potential of $\mathcal{B}_N^{(s-\tau)} \in \mathbb{L}_q(\mathbb{S}^d)$ for $s - d/p > \tau > 0$, so $\mathcal{B}_N^{(s)} \in \mathbb{W}_q^\tau(\mathbb{S}^d)$. The triangle inequality then gives

$$\left\|\mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \leq \left\|\eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} + \left\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)}. \tag{6.3}$$

From (6.1) and (3.8) we deduce the following bound for the polynomial part:

$$\left\|\eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \leq c_{q,\tau,d}\, 2^{m\tau} \left\|\eta_m * \mathcal{B}_N^{(s)}\right\|_q \leq c_{q,\tau,d}\, 2^{m\tau} \|\eta_m\|_{1,d} \left\|\mathcal{B}_N^{(s)}\right\|_q. \tag{6.4}$$

The challenging part is to control the error of approximation $\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)}$. For this purpose we decompose the convolution of η_m against a function $f \in \mathbb{L}_q(\mathbb{S}^d)$,

$$\eta_m * f = \sum_{k=0}^{m} \psi_k * f, \qquad \psi_0 \equiv 1, \quad \psi_k := \psi_{k,h} := B_h^{(0)}(2^{k-1}; \cdot), \quad k \geq 1, \tag{6.5}$$

where h is a filter with support $[1/2, 2]$ and range $[0, 1]$ that also has the property (5.4). We now specify $\widetilde{h}$ in terms of h as follows[2]

$$\widetilde{h}(t) := \begin{cases} 1 & \text{if } t \in [0, 1], \\ h(t) & \text{if } t \geq 1. \end{cases}$$

Then it can be readily verified that

$$\widetilde{h}\left(\frac{\ell}{2^{m-1}}\right) = \sum_{k=1}^{m} h\left(\frac{\ell}{2^{k-1}}\right), \qquad \ell, m \geq 1,$$

which in turn implies (6.5). Furthermore, we note that by [19, Lemma 2.11]

$$\sum_{k=0}^{m} \psi_k * f \to f \qquad \text{as } m \to \infty \text{ in } \mathbb{L}_q(\mathbb{S}^d). \tag{6.6}$$

Now, let $s - d/p > \tau > 0$ and for $\mathbf{x} \in \mathbb{S}^d$ set $\phi^{(s)}(\mathbf{y}) := \mathcal{B}^{(s)}(\mathbf{x} \cdot \mathbf{y})$. First, observe that

$$\mathbf{J}_{-\tau}[\phi^{(s)}] = \phi^{(s-\tau)}, \qquad \mathbf{J}_{-\tau}[\eta_m * \phi^{(s)}] = \eta_m * \mathbf{J}_{-\tau}[\phi^{(s)}] = \eta_m * \phi^{(s-\tau)}.$$

By linearity, these relations also hold for $\mathcal{B}_N^{(s)}$. Hence, by Proposition 3.3,

$$\left\| \mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)} \right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} = \left\| \mathbf{J}_{-\tau}[\mathcal{B}_N^{(s)}] - \mathbf{J}_{-\tau}[\eta_m * \mathcal{B}_N^{(s)}] \right\|_q = \left\| \mathcal{B}_N^{(s-\tau)} - \eta_m * \mathcal{B}_N^{(s-\tau)} \right\|_q.$$

Application of the decomposition relations (6.5) and (6.6) and the triangle inequality gives

$$\left\| \mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)} \right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} = \left\| \sum_{k=m+1}^{\infty} \psi_k * \mathcal{B}_N^{(s-\tau)} \right\|_q \leq \sum_{k=m+1}^{\infty} \left\| \psi_k * \mathcal{B}_N^{(s-\tau)} \right\|_q. \tag{6.7}$$

Defining

$$\psi_k^{(s)} := \psi_k * \phi^{(s)} = B_h^{(s)}(2^{k-1}; \cdot), \qquad k \geq 1, \tag{6.8}$$

we deduce

$$\left\| \psi_k * \mathcal{B}_N^{(s-\tau)} \right\|_q = \left\| \frac{1}{N} \sum_{j=1}^{N} \psi_k^{(s-\tau)}(\mathbf{x}_j \cdot \cdot) \right\|_q \leq \frac{1}{N} \sum_{j=1}^{N} \left\| \psi_k^{(s-\tau)}(\mathbf{x}_j \cdot \cdot) \right\|_q = \left\| B_h^{(s-\tau)}(2^{k-1}; \cdot) \right\|_{q,d}.$$

Lemma 5.2 then yields (since $s - \tau > d/p$ and $2^m \asymp N^{1/d}$)

$$\left\| \mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)} \right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \leq c' \sum_{k=m+1}^{\infty} (2^k)^{d/p-(s-\tau)}$$

$$\leq c'' (2^m)^{d/p-(s-\tau)} \leq c''' N^{1/p-(s-\tau)/d}. \tag{6.9}$$

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[2] The partition of unity property implies smoothness at the transition point $t = 1$. The requirement that $\widetilde{h}$ is 1 on $[0, 1]$ implies that convolution with η_m reproduces a spherical polynomial of degree $\leq 2^{m-1}$.

The upper bound in (6.9) is not strong enough to give the result in Lemma 4.4 except in the case $q = 1$. The following result will enable us to settle the other extremal case $q = \infty$; however, it requires geometric information about the point set.

Lemma 6.2. *Let $s' > d \geq 1$. Then there is a constant c such that for every point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$,*

$$\left| \frac{1}{N} \sum_{j=1}^{N} \psi_k^{(s')}(\mathbf{x}_j \cdot \mathbf{y}) \right| \leq c \left[\gamma(X_N) \right]^d N^{-1} 2^{-k(s'-d)}, \qquad \mathbf{y} \in \mathbb{S}^d; \ k = m, m+1, m+2, \ldots,$$

where $m := \lfloor \frac{1}{d} \log_2 N \rfloor$ and $\psi_k^{(s')}$ is given in (6.8).

Proof. The point set X_N uniquely determines a Voronoi cell decomposition $\{R_1, \ldots, R_N\}$ of $\mathbb{S}^d$ with $\mathbf{x}_j \in R_j$. It has the property that $\min_{1 \leq j \leq N} \sigma_d(R_j) \geq \beta_d \left[\delta(X_N) \right]^d$ for some constant β_d depending only on d. Utilizing a Marcinkiewicz–Zygmund type inequality from [17, Corollary 4.6],

$$\left| \left\| \psi_k^{(s')} \right\|_{1,d} - \sum_{j=1}^{N} \sigma_d(R_j) \left| \psi_k^{(s')}(\mathbf{x}_j \cdot \mathbf{y}) \right| \right| \leq c' \left[2^k \rho(X_N) \right]^d E_{2^{k-1}}(\mathcal{B}^{(s')}), \qquad \mathbf{y} \in \mathbb{S}^d,$$

where $E_n(f) := \inf_{P \in \Pi_n^d} \|f - P\|_1$ is the *error of best $\mathbb{L}_1(\mathbb{S}^d)$-approximation* by spherical polynomials on $\mathbb{S}^d$ of degree at most n, we obtain

$$\left| \sum_{j=1}^{N} \psi_k^{(s')}(\mathbf{x}_j \cdot \mathbf{y}) \right| \leq \frac{1}{\min_{1 \leq j \leq N} \sigma_d(R_j)} \sum_{j=1}^{N} \sigma_d(R_j) \left| \psi_k^{(s')}(\mathbf{x}_j \cdot \mathbf{y}) \right|$$

$$\leq \frac{1}{\min_{1 \leq j \leq N} \sigma_d(R_j)} \left(\left\| \psi_k^{(s')} \right\|_{1,d} + c' \left[2^k \rho(X_N) \right]^d E_{2^{k-1}}(\mathcal{B}^{(s')}) \right).$$

Now, by Lemma 5.2,

$$\left\| \psi_k^{(s')} \right\|_{1,d} = \left\| B_h^{(s')}(2^{k-1}; \cdot) \right\|_{1,d} \leq c'' 2^{-ks'}$$

and proceeding similarly to the derivation of (6.9), we get

$$E_{2^{k-1}}(\mathcal{B}^{(s')}) \leq \left\| \mathcal{B}^{(s')} - \eta_{k-1} * \mathcal{B}^{(s')} \right\|_{1,d} \leq c''' 2^{-ks'}.$$

Hence

$$\left| \sum_{j=1}^{N} \psi_k^{(s')}(\mathbf{x}_j \cdot \mathbf{y}) \right| \leq \frac{c'' 2^{-ks'} + c' \left[2^k \rho(X_N) \right]^d c''' 2^{-ks'}}{\beta_d \left[\delta(X_N) \right]^d}$$

$$= \frac{1}{\beta_d} \left[\frac{\rho(X_N)}{\delta(X_N)} \right]^d \left(\frac{c''}{\left[2^k \rho(X_N) \right]^d} + c' c''' \right) 2^{-k(s'-d)}.$$

The parenthetical expression is bounded because (recalling $k \geq m$) $2^{-k} \leq 2^{-m} \asymp N^{-1/d} \leq c^{iv} \rho(X_N)$. $\quad \square$

Lemma 6.3. *Let $d \geq 1$, $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ and $s - d/p > \tau > 0$, and X_N an N-point set on $\mathbb{S}^d$. Let $m = \lfloor \frac{1}{d} \log_2 N \rfloor$. Then we have*

$$\left\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \le c \left[\gamma(X_N)\right]^{d/p} N^{-(s-\tau)/d}, \tag{6.10}$$

where the constant c depends only on d, p, s and τ.

Proof. The case $q = 1$ is given by (6.9). It suffices to consider the case $q = \infty$, for then the case $1 < q < \infty$ follows from the Riesz–Thorin theorem. By Lemma 6.2,

$$\left\|\psi_k * \mathcal{B}_N^{(s-\tau)}\right\|_\infty = \sup_{\mathbf{y} \in \mathbb{S}^d} \left| \frac{1}{N} \sum_{j=1}^N \psi_k^{(s-\tau)}(\mathbf{x}_j \cdot \mathbf{y}) \right| \le c \left[\gamma(X_N)\right]^d N^{-1} 2^{-k(s-\tau-d)}, \qquad k \ge m,$$

and substitution into (6.7) gives as before

$$\left\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_\infty^\tau(\mathbb{S}^d)} \le \sum_{k=m+1}^\infty \left\|\psi_k * \mathcal{B}_N^{(s-\tau)}\right\|_\infty \le c \left[\gamma(X_N)\right]^d N^{-1} \sum_{k=m+1}^\infty (2^k)^{d-(s-\tau)}$$

$$\le c^{iv} \left[\gamma(X_N)\right]^d N^{-(s-\tau)/d}.$$

This completes the proof. □

We are now ready to prove Lemma 4.4.

Proof of Lemma 4.4. For $N \ge 1$, let $m = \lfloor \frac{1}{d} \log_2 N \rfloor$. First, observe from (6.2) that $\|\mathcal{B}_N^{(s)}\|_q$ is positive. Hence, by (6.3) and (6.4),

$$\left\|\mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \le \left(c_{q,\tau,d} \|\eta_m\|_{1,d} N^{\tau/d} + \frac{\left\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)}}{\left\|\mathcal{B}_N^{(s)}\right\|_q} \right) \left\|\mathcal{B}_N^{(s)}\right\|_q.$$

By Lemma 6.3 and (6.2), the ratio is upper bounded by

$$\left\|\mathcal{B}_N^{(s)} - \eta_m * \mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \Big/ \left\|\mathcal{B}_N^{(s)}\right\|_q \le \frac{c \left[\gamma(X_N)\right]^{d/p} N^{(\tau-s)/d}}{c'_{p,s,d} N^{-s/d}} = c'' \left[\gamma(X_N)\right]^{d/p} N^{\tau/d}.$$

Therefore

$$\left\|\mathcal{B}_N^{(s)}\right\|_{\mathbb{W}_q^\tau(\mathbb{S}^d)} \le \left(c_{q,s,d} \|\eta_m\|_{1,d} + c'' \left[\gamma(X_N)\right]^{d/p} \right) N^{\tau/d} \left\|\mathcal{B}_N^{(s)}\right\|_q.$$

The result follows by observing with the aid of Lemma 3.5 that $\|\eta_m\|_{1,d}$ is bounded uniformly in m. □

7. Example: the unit circle

In order to gain more insight into the covering problem, we turn to the unit circle $\mathbb{S} := \mathbb{S}^1$ and exploit the fact that this one-dimensional manifold is more accessible than its higher-dimensional counterparts and appeal at the same time to the general principle that certain fundamental features are shared across changing dimensions. Circular designs (i.e. equally spaced points) on $\mathbb{S}$ are exact for all trigonometric polynomials with degree strictly less than the number of points. They form QMC-design sequences, that is, give rise to optimal order worst-case error for QMC methods that integrate functions from the Sobolev space $\mathbb{W}_p^s(\mathbb{S})$ for

every $p \geq 1$ and every $s > 1/p$. One question then is: *How much of the QMC-design property is destroyed when just one point is removed from each configuration?*

We interpret $\mathbb{W}_p^s(\mathbb{S})$ as a Bessel potential space (see Section 3).[3] The Bessel kernel for $\mathbb{S}$ then reduces to the Fourier cosine series

$$\mathcal{B}^{(s)}(\cos\phi) = B^{(s)}(\cos\phi) - 1 = 2 \sum_{\ell=1}^{\infty} \frac{\cos(\ell\phi)}{(1+\ell^2)^{s/2}}. \tag{7.1}$$

The $\mathbb{L}_q(\mathbb{S})$-norm of $B^{(s)}$ is bounded if $s > 1/p$ with $1/q + 1/p = 1$ (Lemma 3.5). The worst-case error of $Q[X_N]$ of a node set $X_N \subset \mathbb{S}$ can then be expressed in terms of an appropriate Bessel kernel (see Theorem 4.1 and the remark following this theorem). For the asymptotic analysis of the worst-case error we express the Bessel kernel in terms of generalized Clausen functions; i.e.,[4]

$$\mathcal{B}^{(s)}(\cos\phi) = 2\,\mathrm{Ci}_s(\phi) + 2 \sum_{m=1}^{\infty} (-1)^m \frac{(s/2)_m}{m!}\,\mathrm{Ci}_{s+2m}(\phi), \tag{7.2}$$

where for $\mathrm{Re}\, z > 1$ the *generalized Clausen cosine* and *sine functions* are defined as

$$\mathrm{Ci}_z(\phi) := \sum_{\ell=1}^{\infty} \frac{\cos(\ell\,\phi)}{\ell z}, \qquad \mathrm{Si}_z(\phi) := \sum_{\ell=1}^{\infty} \frac{\sin(\ell\,\phi)}{\ell z},$$

which may be extended to the complex z-plane by analytic continuation.

Remark. By mapping the unit circle to the interval $[0, 1)$, the functions in $\mathbb{W}_p^s(\mathbb{S})$ become Fourier series

$$f(x) = \sum_{k \in \mathbb{Z}} \widehat{f}(k)\,\mathrm{e}^{2\pi\mathrm{i}kx}.$$

In the Hilbert space setting ($p = 2$), a slight modification of the coefficients in (7.1) ($(1+\ell^2)^{-s/2}$ is changed to $r_s(0) := 1$ and $r_s(\ell) := |\ell|^{-s}$ for $\ell \geq 1$), gives the standard Korobov space [28], which is a reproducing kernel Hilbert space with reproducing kernel

$$K_s(x, y) = \sum_{\ell \in \mathbb{Z}} r_s(\ell)\,\mathrm{e}^{2\pi\mathrm{i}\ell(x-y)} = 1 + 2 \sum_{\ell=1}^{\infty} \frac{\cos(2\pi\ell(x-y))}{\ell^s}.$$

Since $\ell^s \leq (1+\ell^2)^{s/2} \leq 2^{s/2}\ell^s$ for $\ell \geq 1$, we have that the change of coefficients yields a space with equivalent norm. Numerical integration in (tensor-product) Korobov spaces is discussed in many papers, see [11, Section 5].

It is natural to study the Hilbert space setting (when $p = 2$) and the general non-Hilbert space setting (when $p \geq 1$), separately.

7.1. Hilbert space setting

As described in [9], the *strength* (more precisely, the *2-strength*) of a sequence (X_N) of N-point sets on $\mathbb{S}$ is the supremum of the indices $s \geq 1/2$ for which (X_N) is a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$. In particular, the 2-strength of a sequence of circular designs X_N with N equally spaced points as $N \to \infty$ is infinite.

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[3] Alternatively, for $p = 2$ one can use the approach in [9].
[4] We use the *Pochhammer symbol* to denote rising factorials: $(a)_0 := 1$, $(a)_{n+1} := (n + a)(a)_n$.

Theorem 7.1. *Let $s > 1/2$. A sequence of configurations of N equally spaced points after one point is removed (or a uniformly bounded number of points are removed) from each configuration is a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ for every $1/2 < s \leq 1$ but not for $s > 1$; i.e., such a sequence has 2-strength 1.*

Proof. Let $s > 1/2$. Then the Bessel kernel $B^{(2s)}$ is a reproducing kernel for the Bessel potential space $\mathbb{W}_2^s(\mathbb{S})$ and by the reproducing kernel Hilbert space approach the squared worst-case error of $Q[X_N]$ of a node set $X_N = \{(\cos\phi_j, \sin\phi_j)\}_{j=0}^{N-1} \subset \mathbb{S}$ has the form

$$[\text{wce}(Q[X_N]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \mathcal{B}^{(2s)}(\cos(\phi_j - \phi_k)). \tag{7.3}$$

Let the points in X_N be the equally spaced Nth roots of unity so that $\phi_j = 2\pi j/N$, $j = 0, \ldots, N-1$. Such points are circular $(N-1)$-designs and satisfy the following identities: let $\ell = 0, 1, 2, \ldots$, then

$$\sum_{k=0}^{N-1} \sin\frac{2\pi\ell k}{N} = 0, \qquad \sum_{k=0}^{N-1} \cos\frac{2\pi\ell k}{N} = \begin{cases} N & \text{if } N \mid \ell, \\ 0 & \text{if } N \nmid \ell, \end{cases} \tag{7.4}$$

where $N \mid \ell$ means that ℓ is an integer multiple of N ("N divides ℓ") and $N \nmid \ell$ means that ℓ is not divisible by N. Substituting (7.2) into the worst-case error formula (7.3) and using (7.4), straightforward computation gives

$$\text{wce}(Q[X_N]; \mathbb{W}_2^s(\mathbb{S})) = \frac{1}{N^s} \left(2\zeta(2s) + \sum_{m=1}^{\infty} (-1)^m \frac{(s)_m}{m!} \frac{2\zeta(2s+2m)}{N^{2m}} \right)^{1/2}; \tag{7.5}$$

i.e., we recover the fact that equally spaced points, indeed, form QMC-design sequences for $\mathbb{W}_2^s(\mathbb{S})$ for each $s > 1/2$.

Now, let Z_{N-M} denote the collection of Nth roots of unity with the first M points omitted. Using (7.4), it is readily verified that

$$\sum_{k=M}^{N-1} \mathcal{B}^{(2s)}\left(\cos\left(\frac{2\pi k}{N} - \phi\right)\right) = 2N \sum_{\nu=1}^{\infty} \frac{\cos(N\phi)}{(1 + \nu^2 N^2)^s} - \sum_{k=0}^{M-1} \mathcal{B}^{(2s)}\left(\cos\left(\frac{2\pi k}{N} - \phi\right)\right). \tag{7.6}$$

Substituting into the worst-case error formula (7.3), we get

$$[\text{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{1}{(N-M)^2} \sum_{j=M}^{N-1} \sum_{k=M}^{N-1} \mathcal{B}^{(2s)}\left(\cos\left(\frac{2\pi k}{N} - \frac{2\pi j}{N}\right)\right)$$

$$= \frac{2N(N-M)}{(N-M)^2} \sum_{\nu=1}^{\infty} \frac{1}{(1 + \nu^2 N^2)^s} - \frac{1}{(N-M)^2} \sum_{k=0}^{M-1} \sum_{j=M}^{N-1} \mathcal{B}^{(2s)}\left(\cos\left(\frac{2\pi j}{N} - \frac{2\pi k}{N}\right)\right).$$

A second application of (7.6) gives

$$[\text{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{2N(N-2M)}{(N-M)^2} \sum_{\nu=1}^{\infty} \frac{1}{(1 + \nu^2 N^2)^s} + \frac{M^2}{(N-M)^2} \mathcal{B}_{N,M}^{(2s)},$$

where

$$\mathcal{B}_{N,M}^{(2s)} := \frac{1}{M^2} \sum_{j=0}^{M-1} \sum_{k=0}^{M-1} \mathcal{B}^{(2s)}\left(\cos\frac{2\pi(j-k)}{N}\right)$$

$$= \mathcal{B}^{(2s)}(1) - \frac{2}{M^2} \sum_{\nu=1}^{M-1}(M-\nu)\left[\mathcal{B}^{(2s)}(1) - \mathcal{B}^{(2s)}\left(\cos\frac{2\pi\nu}{N}\right)\right]$$

and

$$\mathcal{B}^{(2s)}(1) = 2\sum_{m=0}^{\infty}(-1)^m\frac{(s)_m}{m!}\zeta(2s+2m) = 2\sum_{\ell=1}^{\infty}\frac{1}{(1+\ell^2)^{s/2}}. \tag{7.7}$$

Observe from (7.1) that the square-bracketed expression above is non-negative. Furthermore, one has

$$0 \le \mathcal{B}^{(2s)}(1) - \mathcal{B}_{N,M}^{(2s)} \le \left(\frac{2}{M^2}\sum_{\nu=1}^{M-1}(M-\nu)\right) \max_{0\le x\le 2\pi M/N}\left[\mathcal{B}^{(2s)}(1) - \mathcal{B}^{(2s)}\left(\cos\frac{2\pi\nu}{N}\right)\right].$$

Since the parenthetical expression is bounded by 1 and the maximum tends to zero when $M/N \to 0$, we arrive at

$$[\mathrm{wce}(\mathrm{Q}[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{2N(N-2M)}{(N-M)^2}\sum_{\nu=1}^{\infty}\frac{1}{(1+\nu^2 N^2)^s} + \frac{M^2}{(N-M)^2}\left\{\mathcal{B}^{(2s)}(1) + o(1)\right\}.$$

Rewriting the infinite series, we finally arrive at

$$[\mathrm{wce}(\mathrm{Q}[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{M^2}{(N-M)^2}\left\{\mathcal{B}^{(2s)}(1) + \cdots\right\} + \frac{N(N-2M)}{(N-M)^2}\left\{\frac{2\zeta(2s)}{N^{2s}} + \cdots\right\}$$

Let $M = 1$. Then for $1/2 < s < 1$ we obtain the asymptotics

$$\mathrm{wce}(\mathrm{Q}[Z_{N-1}]; \mathbb{W}_2^s(\mathbb{S})) = \frac{\sqrt{2\zeta(2s)}}{(N-1)^s}\left\{1 + \frac{\mathcal{B}^{(2s)}(1)}{4\zeta(2s)}(N-1)^{2s-2} + \cdots\right\},$$

whereas for $s > 1$ we have that

$$\mathrm{wce}(\mathrm{Q}[Z_{N-1}]; \mathbb{W}_2^s(\mathbb{S})) = \frac{\sqrt{\mathcal{B}^{(2s)}(1)}}{N-1}\left\{1 + \frac{\zeta(2s)}{\mathcal{B}^{(2s)}(1)}(N-1)^{2-2s} + \cdots\right\}.$$

We conclude that (Z_{N-1}) is a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ if and only if $1/2 < s \le 1$; i.e., the 2-strength of (Z_{N-1}) is 1. This completes the proof when one point is omitted. $\square$

A similar but more tedious argument provides the leading term behavior of the asymptotics of the worst-case error when a finite number (uniformly upper bounded) of points are removed from a circular design.

Let Z_{N-M} denote a configuration of N equally spaced points on $\mathbb{S}$ with M consecutive points removed. The hole thus generated in Z_{N-M} has covering radius

$$\rho(Z_{N-M}) = \frac{\pi(M+1)}{N}. \tag{7.8}$$

(Note that π/N is the packing radius of the N equally sized circular arcs making up $\mathbb{S}$ which is half of the minimal geodesic separation distance of points in Z_{N-M}.) For our discussion we want to assume that the

hole size shrinks as N grows, so $M/N \to 0$ as $N \to \infty$. Theorem 7.1 covers the case when M is uniformly bounded. We now consider the case $M \to \infty$ which is equivalent to $N\rho(Z_{N-M}) \to \infty$ as $N \to \infty$. Then the sequence (Z_{N-M}) does not have the optimal covering property. The next theorem shows that, despite bad covering, (Z_{N-M}) has 2-strength 1 if the artificially generated holes shrink rapidly enough. Interestingly, the sequence (Z_{N-M}) is **not** a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ for $s = 1$. Moreover, if the hole size shrinks too slowly, then (Z_{N-M}) is not a QMC-design sequence for any $s > 1/2$. However, one can choose the asymptotic behavior of the covering radius to get as close as one likes to a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ for $1/2 < s < 1$ (e.g., when the covering radius behaves like $(\log \circ \cdots \circ \log N)/N^s$).

Theorem 7.2. *Let $s > 1/2$ and (Z_{N-M}) be as above with $M \to \infty$ and $M/N \to 0$.*

(a) *If $N^s \rho(Z_{N-M}) \to c$ for some real $c \geq 0$, then (Z_{N-M}) has 2-strength 1 but is not a QMC-design sequence for $s = 1$.*
(b) *If $N^s \rho(Z_{N-M}) \to \infty$, then (Z_{N-M}) is not a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ with $s > 1/2$. In particular, when $1/2 < s < 3/2$,*

$$\mathrm{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S})) = \sqrt{\mathcal{B}^{(2s)}(1)} \, \frac{\rho(Z_{N-M})}{\pi} \{1 + o(1)\} \qquad as \ N \to \infty,$$

where $\mathcal{B}^{(2s)}(1)$ is the constant in (7.7).

Proof. We proceed along the same lines as the proof of Theorem 7.1 and determine the asymptotic (large N) behavior of the worst-case error for QMC methods based on node sets Z_{N-M} for functions in $\mathbb{W}_2^s(\mathbb{S})$ with $s > 1/2$. Let Z_{N-M} denote the collection of Nth roots of unity with the first M points omitted. For $M/N \to 0$ as $N \to \infty$, we obtained the following asymptotics in the proof of Theorem 7.1:

$$[\mathrm{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S}))]^2 = \frac{M^2}{(N-M)^2} \left\{ \mathcal{B}^{(2s)}(1) + \cdots \right\} + \frac{N(N-2M)}{(N-M)^2} \left\{ \frac{2\zeta(2s)}{N^{2s}} + \cdots \right\}.$$

Now, let M grow with N such that $M/N \to 0$ and $M \to \infty$ as $N \to \infty$. The unboundedness of M implies that $N\rho(Z_{N-M}) = \pi(M + 1) \to \infty$ as $N \to \infty$ and thus (Z_{N-M}) does not have the optimal covering property. However, for $N^s M/(N-M) \to c$ as $N \to \infty$ for some real $c \geq 0$, we still have that

$$\mathrm{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S})) = \frac{\left(2\zeta(2s) + c^2 \mathcal{B}^{(2s)}(1)\right)^{1/2}}{N^s} \{1 + o(1)\} \qquad as \ N \to \infty,$$

where $\mathcal{B}^{(2s)}(1)$ is given in (7.7). Thus (Z_{N-M}) is a QMC-design sequence for $\mathbb{W}_2^s(\mathbb{S})$ for $1/2 < s < 1$. (The upper bound on s is imposed by the unboundedness of M.) On the other hand, when $N^s M/(N-M) \to \infty$, then

$$\mathrm{wce}(Q[Z_{N-M}]; \mathbb{W}_2^s(\mathbb{S})) = \sqrt{\mathcal{B}^{(2s)}(1)} \, \frac{M}{N-M} \{1 + o(1)\} \qquad as \ N \to \infty.$$

The last convergence relation for M is automatically satisfied for $s \geq 1$ and gives a suboptimal convergence rate for the worst-case error when $1/2 < s < 3/2$. The result follows by using the covering radius instead of M (see (7.8)). $\square$

7.2. The general case $p \geq 1$

We now leave the Hilbert space setting and consider $\mathbb{W}_p^s(\mathbb{S})$ for $p \geq 1$. Let $s > 1/p$. By Theorem 4.1 the worst-case error for $Q[Z_N]$ for a circular design consisting of the Nth roots of unity for $\mathbb{W}_p^s(\mathbb{S})$ is

given by the $\mathbb{L}_q(\mathbb{S})$-norm of the function $\mathcal{B}_N^{(s)}$ of (4.2). On the unit circle one can write with the help of (7.6),

$$\mathcal{B}_N^{(s)}(\cos\phi) = \frac{1}{N}\sum_{k=0}^{N-1}\mathcal{B}^{(s)}\left(\cos\left(\frac{2\pi k}{N}-\phi\right)\right) = \frac{2}{N^s}\sum_{\nu=1}^{\infty}\frac{\cos(N\phi)}{(\nu^2+1/N^2)^{s/2}}.$$

Hence

$$\mathrm{wce}(\mathrm{Q}[Z_N];\mathbb{W}_p^s(\mathbb{S})) = \left\|\mathcal{B}_N^{(s)}\right\|_q = \frac{2}{N^s}\left(\frac{1}{2\pi}\int_0^{2\pi}\left|\sum_{\nu=1}^{\infty}\frac{\cos(N\phi)}{(\nu^2+1/N^2)^{s/2}}\right|^q\mathrm{d}\phi\right)^{1/q}.$$

Dividing the integration domain into N parts and using the 2π-periodicity of the integrand, it follows that

$$\mathrm{wce}(\mathrm{Q}[Z_N];\mathbb{W}_p^s(\mathbb{S})) = \frac{2}{N^s}\left(\frac{1}{2\pi}\int_0^{2\pi}\left|\sum_{\nu=1}^{\infty}\frac{\cos\phi}{(\nu^2+1/N^2)^{s/2}}\right|^q\mathrm{d}\phi\right)^{1/q}.$$

For large N, the series can be approximated by the generalized Clausen cosine function. A mean value argument $((x^2+\varepsilon)^{q/2} = |x|^q + \frac{1}{2}q\varepsilon(x^2+\varepsilon')^{q/2-1}$ for $0 < \varepsilon' < \varepsilon)$ gives that

$$\mathrm{wce}(\mathrm{Q}[Z_N];\mathbb{W}_p^s(\mathbb{S})) = \frac{2}{N^s}\left(\frac{1}{2\pi}\int_0^{2\pi}|\mathrm{Ci}_s(\phi)|^q\,\mathrm{d}\phi + \mathcal{O}(N^{-2})\right)^{1/q} \qquad \text{as } N\to\infty. \tag{7.9}$$

Let Z_{N-M} be the set of Nth roots of unity with M consecutive points omitted. Then (7.6) gives that

$$\mathcal{B}_{N-M}^{(s)}(\cos\phi) = \frac{1}{N-M}\sum_{k=1}^{N-M}\mathcal{B}^{(s)}\left(\cos\left(\frac{2\pi k}{N}-\phi\right)\right)$$

$$= \frac{N}{N-M}\frac{2}{N^s}\sum_{\nu=1}^{\infty}\frac{\cos(N\phi)}{(\nu^2+1/N^2)^{s/2}} - \frac{1}{N-M}\sum_{k=0}^{M-1}\mathcal{B}^{(s)}\left(\cos\left(\frac{2\pi k}{N}-\phi\right)\right).$$

Similarly as before, we get

$$\mathrm{wce}(\mathrm{Q}[Z_{N-M}];\mathbb{W}_p^s(\mathbb{S})) = \left(\frac{1}{N}\sum_{k=0}^{N-1}\int_0^1\left|\frac{N}{N-M}\frac{2}{N^s}\sum_{\nu=1}^{\infty}\frac{\cos(2\pi x)}{(\nu^2+1/N^2)^{s/2}}\right.\right.$$

$$\left.\left. - \frac{1}{N-M}\sum_{j=0}^{M-1}\mathcal{B}^{(s)}\left(\cos\frac{2\pi(x+k-j)}{N}\right)\right|^q\mathrm{d}x\right)^{1/q}.$$

Approximation with a generalized Clausen cosine function gives

$$\mathrm{wce}(\mathrm{Q}[Z_{N-M}];\mathbb{W}_p^s(\mathbb{S})) = \left(\frac{1}{N}\sum_{k=0}^{N-1}\int_0^1\left|\frac{N}{N-M}\frac{2\,\mathrm{Ci}_s(2\pi x)+\mathcal{O}(N^{-2})}{N^s}\right.\right.$$

$$\left.\left. - \frac{M}{N-M}\frac{1}{M}\sum_{j=0}^{M-1}\mathcal{B}^{(s)}\left(\cos\frac{2\pi(x+k-j)}{N}\right)\right|^q\mathrm{d}x\right)^{1/q}.$$

The asymptotic behavior of the worst-case error is determined by the limiting behavior of $N^s\rho(Z_{N-M})$ as $N \to \infty$. Similar results to the Hilbert space setting can be derived. We leave this to the reader. (Particular care is needed when both contributions between the absolute value signs are in "balance" for large N; e.g., when $M = 1$ and $s = 1$.)

Acknowledgments

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