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Original Research Paper

CONFIDENCE BOUNDS FOR SPHERICAL SAMPLING SCHEMES IN STEREOLOGY

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ABSTRACT

This paper considers quadrature methods for integration over the unit sphere using reproducing kernel Hilbert spaces. Bayesian quadrature weights, which minimize the worst-case integration error, and their normalized counterparts, which additionally integrate constants exactly, are studied. Deterministic error bounds are established in terms of the Sobolev regularity of the integrand and geometric properties of the sampling design. For designs obtained by applying a uniformly random rotation to a fixed point configuration, exact mean and bias identities are derived, and the variance is bounded by the squared worst-case error. The normalized estimator is unbiased, whereas the bias of the unconstrained Bayesian estimator is proportional to its squared worst-case error. To construct data-dependent bounds, an ordinary least-squares estimator of the spherical harmonic coefficients is introduced, yielding a conservative 95% confidence interval under an assumption on the Sobolev norm of the harmonic tail. The framework is applied to the Nucleator in stereology, for which explicit error bounds are obtained for convex bodies in dimensions two and three.

Keywords: Nucleator; Reproducing kernel Hilbert spaces; Spherical quadrature; Stereology.

INTRODUCTION

In this paper we are interested in estimating the integral of an integrable function f over the Euclidean sphere $S^{n-1} = \{x \in \mathbb{R}^n : \|x\| = 1\}$, that is

$$I(f) = \int_{S^{n-1}} f(u)\, \mathscr{H}^{n-1}(du), \tag{1.1}$$

where $\mathscr{H}^{n-1}$ is the $(n-1)-$dimensional Hausdorff measure on $\mathbb{R}^n$. We use the normalization $\mathscr{H}^{n-1}(S^{n-1}) = \omega_{n-1}$, with ω_{n-1} the surface area of the sphere S^{n-1}. We aim to estimate the integral in (1.1) by an estimator of the form

$$\widehat{V}_w(f;X) = \sum_{x\in X} w(x,X) f(x), \tag{1.2}$$

where $X = \{x_1,\dots,x_N\} \subset S^{n-1}$ is finite and $W(X) = (w(x_1,X),\dots,w(x_N,X))$ is the weight vector.

A motivation of estimating integrals comes from Stereology. For instance, consider the *nucleator*. If $K \subset \mathbb{R}^n$ is star-shaped with respect to the origin and ρ_K denotes its radial function, then its volume can be written as a spherical integral of ρ_K^n, and thus fits into the framework, see (Gundersen, 1988) for the case $n = 3$.

We aim to consider quadrature rules on S^{n-1} that provide deterministic error control. The present approach is related to the one-dimensional Newton–Cotes theory developed in the papers Stehr and Kiderlen (2020a;b; 2025) for estimating integrals over $\mathbb{R}$. They fit the weights using exactness of integration of polynomials of a fixed degree. In Stehr and Kiderlen (2025) asymptotic 100% confidence intervals for the Newton–Cotes estimator are derived, where the width is essentially controlled by the number of sampling points and differentiability assumptions on the function, see Stehr and Kiderlen (2025, Thm. 2). The consideration of 100% confidence intervals instead of $1-\alpha$ confidence intervals is motivated by the work presented in Christensen (2020); García-Fiñana (2006). Herein, the Cavalieri estimator on $\mathbb{R}^1$ is considered and it is shown that limit distributions of the standardized Cavalieri estimator only exist in special cases depending on the function involved.

In the present paper, we use *reproducing kernel Hilbert spaces* (RKHS) on the sphere to define two quadrature systems. We consider Bayesian quadrature weights $W_*(X)$, which minimize the worst-case integration error, and normalized weights $W_0(X)$, which minimize the worst-case integration error under the constraint of preserving exact integration of constants. The resulting error bounds depend on a suitable norm of the integrand and on geometric quantities of the design, such as fill distance and mesh ratio. This is the spherical counterpart of the results in Soto (2025), where they consider integration on the torus $\mathbb{T}^n = \mathbb{R}^n/T\mathbb{Z}^n$ for $T > 0$ using reproducing kernel Hilbert spaces. On this, we remark that the only overlap is the one-dimensional setup as $\mathbb{T}^1$ is homeomorphic to S^1, while for $n > 1$

the sphere differs from the torus, see Hatcher (2002, Chap. 1).

We deliberately describe the problem in deterministic terms, and keep the stochastic component narrow, and note that without much alteration most results can be framed in a more stochastic setup. To illustrate this, we introduce *rotational designs* as a simple motivating example of how to translate to a stochastic setting. We define this stochastic point process on the sphere by $X_R = RX_0$, where $X_0 \subset S^{n-1}$ is fixed and R is a stochastic rotation in $\mathbb{R}^n$ with a distribution that is invariant under rotations. This is the natural spherical analogue in S^{n-1} of a uniform random shift of a deterministic systematic design in $\mathbb{R}^n$. For rotational designs, we show, how the deterministic quadrature theory yields exact mean and bias identities, variance bounds, and pathwise 100% error intervals.

A central part of this paper is establishing convergence rates for the error $|I(f) - \widehat{V}_w(f;X)|$ for the two quadrature weights W_* and W_0, see Theorem 2.1 and Corollary 2.2. Related results were obtained by Fuselier *et al.* (2014); Kanagawa *et al.* (2020), which we compare with our setting immediately before Theorem 2.1.

As an application of the theory, we consider the Nucleator in dimensions two and three. By imposing geometric constraints on the radial function of the underlying convex body, we obtain explicit pathwise 100% error bounds, holding uniformly over the specified classes of convex bodies. This differs from previous studies of the Nucleator, such as González-Villa *et al.* (2017), who investigate the precision of systematic sampling and associated variance predictors, and Gomez-Perez *et al.* (2019), who use RKHS on the torus $\mathbb{T}^2$ for variance prediction. They also suggest using reproducing kernel Hilbert spaces directly on the sphere, as done in the present manuscript (Gomez-Perez *et al.*, 2019, p. 141).

The paper is organized as follows. Section 2 contains the main content on deterministic bounds using RKHS theory. First, we introduce the notation needed, and then, we introduce the RKHS framework and prove deterministic error bounds for the weights W_* and W_0 and rates of decay. Section 3 treats systematic random rotations and considers, bias, variance statements, and a conservative 95% confidence interval for the error. We end this section and the paper by applying the theory to the Nucleator on S^1 and S^2.

PRELIMINARIES IN A DETERMINISTIC FRAMEWORK

We begin by fixing notation. Let $\mathrm{SO}(n)$ denote the group of proper rotations of $\mathbb{R}^n$, equipped with the unique Haar probability measure ν, see Schneider and Weil (2008). For $R \in \mathrm{SO}(n)$ and $X \subset S^{n-1}$, we write $RX = \{Rx : x \in X\}$ for the point-wise rotation of the set X by R. If R has distribution ν and $X_0 \subset S^{n-1}$ is considered fixed, the random set $X_R = RX_0$ will be denoted a *rotational design*. In this paper, we consider the space $L^2(S^{n-1})$ (and subset thereof) of square integrable real valued functions on the sphere endowed with the measure $\mathscr{H}^{n-1}$. From Atkinson and Han (2012, Thm. 2.38) it follows that $L^2(S^{n-1})$ admits the orthogonal decomposition

$$L^2(S^{n-1}) = \bigoplus_{k=0}^{\infty} \mathbb{Y}_k^n, \tag{2.1}$$

where $\mathbb{Y}_k^n$ is the space of spherical harmonics of order k in n dimensions together with $f \equiv 0$. The dimension $N_{k,n}$ of $\mathbb{Y}_k^n$ is finite (Atkinson and Han, 2012, p. 18), and for an orthonormal basis $\{Y_{k,j} : j = 1, \ldots, N_{k,n}\}$ of $\mathbb{Y}_k^n$, the addition theorem gives

$$\sum_{j=1}^{N_{k,n}} Y_{k,j}(x)\overline{Y_{k,j}(y)} = \frac{N_{k,n}}{\omega_{n-1}} P_{k,n}(x \cdot y), \quad x, y \in S^{n-1} \tag{2.2}$$

with $P_{k,n}$ the Legendre polynomial defined in Atkinson and Han (2012, eq. (2.19)), $x \cdot y$ denoting the usual inner product between two elements $x, y \in S^{n-1}$, and $\omega_{n-1} = 2\pi^{\frac{n}{2}}/\Gamma(n/2)$ matching the notation from Narcowich *et al.* (2007). We remark that a Fourier type decomposition of $f \in L^2(S^{n-1})$ is given by

$$f = \sum_{k=0}^{\infty} \sum_{j=1}^{N_{k,n}} \hat{f}_{k,j} Y_{k,j} \tag{2.3}$$

with $\hat{f}_{k,j} = \langle f, Y_{k,j} \rangle_{L^2}$. We, as in Atkinson and Han (2012); Narcowich *et al.* (2007), define for $s > (n-1)/2$, the Sobolev space

$$\mathbb{H}^s = \left\{ f \in L^2(S^{n-1}) : \sum_{k=0}^{\infty} (1+\lambda_k)^s \sum_{j=1}^{N_{k,n}} |\widehat{f}_{k,j}|^2 < \infty \right\}, \tag{2.4}$$

where $-\lambda_k = -k(k+n-2)$ corresponds to the Laplace–Beltrami eigenvalue of $\mathbb{Y}_k^n$ for $k \in \mathbb{N}_0$. The inner product on $\mathbb{H}^s(S^{n-1})$ is given by

$$\langle f, g \rangle_{\mathbb{H}^s} = \sum_{k=0}^{\infty} (1+\lambda_k)^s \sum_{j=1}^{N_{k,n}} \widehat{f}_{k,j} \widehat{g}_{k,j}. \tag{2.5}$$

We remark, that the Laplace-Beltrami operator $\Delta_{S^{n-1}}$ can be used to yield another representation of the norm $\|\cdot\|_{\mathbb{H}_s}$, than the one given in (2.4) for $s \in \mathbb{N}_0$. Indeed, since $-\Delta_{S^{n-1}} Y_{k,j} = \lambda_k Y_{k,j}$ (Atkinson and Han, 2012, Prop. 3.5), we can define the operator $(-\Delta_{S^{n-1}})^{\ell/2}$ for $\ell \in \mathbb{N}$ by

$$(-\Delta_{S^{n-1}})^{\ell/2} f = \sum_{k=0}^{\infty} \sum_{j=1}^{N_{k,n}} \lambda_k^{\ell/2} \widehat{f}_{k,j} Y_{k,j},$$

valid for f such that the right hand side converges, for instance if $f \in \mathbb{H}^s$ with $s > \ell$. If $s \in \mathbb{N}_0$, then orthonormality of the spherical harmonics and the binomial theorem give

$$\|f\|^2_{\mathbb{H}^s(S^{n-1})} = \sum_{\ell=0}^{s} \binom{s}{\ell} \|(-\Delta_{S^{n-1}})^{\ell/2} f\|^2_{L^2(S^{n-1})}. \quad (2.6)$$

This alternative representation will be used towards the end of this paper. The space $\mathbb{H}^s$ is continuously embedded in $C(S^{n-1})$ and is a reproducing kernel Hilbert space with kernel

$$K_s(x,y) = \sum_{k=0}^{\infty} (1+\lambda_k)^{-s} \sum_{j=1}^{N_{k,n}} Y_{k,j}(x) Y_{k,j}(y), \quad (2.7)$$

for $x, y \in S^{n-1}$; see (Narcowich *et al.*, 2007, p. 374). By the addition theorem, K_s is a kernel obtained by weighting kernels of the finite harmonic spaces $\mathbb{Y}_k^n$ with the factors $(1+\lambda_k)^{-s}$, that is

$$\begin{aligned} K_s(x,y) &= \Phi_s(x \cdot y), \\ \Phi_s(t) &= \sum_{k=0}^{\infty} (1+\lambda_k)^{-s} \frac{N_{k,n}}{\omega_{n-1}} P_{k,n}(t), \end{aligned} \quad (2.8)$$

so K_s is invariant under simultaneous rotations of x and y. Other weights than $(1+\lambda_k)^{-s}$ in (2.7) could have been used in the definition of K_s. As a kernel uniquely determines a reproducing kernel Hilbert space (Leobacher and Pillichshammer, 2014) one could wonder if other spaces than $\mathbb{H}^s$ fit into the framework to come. We opt out of this discussion and remark that if the weights asymptotically equal $(1+\lambda_k)^{-s}$, then the corresponding space is $\mathbb{H}^s$, compare Soto (2025, Example 3) and Narcowich *et al.* (2007). Lastly, note that

$$\int_{S^{n-1}} K_s(u,x)\, \mathscr{H}^{n-1}(du) = 1, \qquad x \in S^{n-1}, \quad (2.9)$$

We will now show how reproducing kernel Hilbert space can be used to provide bounds for the integration error.
Given a finite point set $X = \{x_1, \ldots, x_N\} \subset S^{n-1}$ we estimate the integral $I(f)$ in (1.1) by estimators of the form (1.2). Our approach mimics the one in Soto (2025), and we refer to this for further arguments in derivations of the next few equations.
We view the integral $I(f)$ as a linear operator $I : \mathbb{H}^s \mapsto \mathbb{R}$, where its Riesz representer is the constant function 1. Using the reproducing kernel property of (2.7) and Cauchy–Schwarz inequality, we get an upper bound for the integration error

$$\begin{aligned} &|I(f) - \hat{V}_w(f;X)| \\ &\qquad \le \|f\|_{\mathbb{H}^s} \left\| 1 - \sum_{x \in X} w(x,X)\, K_s(x,\cdot) \right\|_{\mathbb{H}^s}. \end{aligned} \quad (2.10)$$

We then define the *worst–case* error as

$$e_s(X,w) = \sup_{\|f\|_{\mathbb{H}^s} \le 1} |I(f) - \hat{V}_w(f;X)|.$$

Alternatively, by (2.9) and (2.10) we have

$$e_s(X,w)^2 = \omega_{n-1} - 2w^T \mathbf{1} + w^T K_s w, \quad (2.11)$$

where $K_s(X)$ is a matrix of dimensions $N \times N$ with entries $K_s(X)_{i,j} = K_s(x_i, x_j)$.

To minimize the integration error, we want weights that minimize (2.11). Weights w minimizing (2.11) satisfy the linear system

$$K_s(X) w = \mathbf{1}. \quad (2.12)$$

For distinct points, $K_s(X)$ is positive definite, so in this case the solution to (2.12) is unique and given by

$$W_*^s(X) = K_s(X)^{-1} \mathbf{1}. \quad (2.13)$$

We refer to $W_*^s(X)$ as the Bayesian quadrature weights, since they coincide with the posterior-mean quadrature weights obtained by placing a Gaussian process prior with covariance kernel K on the integrand, see O'Hagan (1991) or Karvonen *et al.* (2019, eq. 3).

Later, we will encounter a setting, where the Bayesian quadrature weights simplifies. We remark, that if $\mathbf{1}$ is an eigenvector of $K_s(X)$ with eigenvalue $\gamma_X \neq 0$, then $K_s(X)\left(1/\gamma_X \mathbf{1}\right) = \mathbf{1}$, and by uniqueness $W_*^s(X) = \left(\frac{1}{\gamma_X}\mathbf{1}\right)$. In the present paper we will also consider the normalized version of the Bayesian quadrature rule, which we denote by

$$W_0^s(X) = \omega_{n-1} \frac{W_*^s(X)}{W_*^s(X)^T \mathbf{1}}. \quad (2.14)$$

These minimize $e_s(X,w)$ under the constraint $w^\top \mathbf{1} = \omega_{n-1}$. These two weights are the main focus of this paper, and we remark that both are rotational invariant and if $X \subset S^{n-1}$ is finite with pairwise distinct points,

then it can be shown by inserting (2.13) or (2.14) into (2.11), that

$$e_s(X, W_*^s(X))^2 = \omega_{n-1} - \mathbf{1}^\top W_*^s(X), \tag{2.15}$$

$$e_s(X, W_0^s(X))^2 = \frac{\omega_{n-1}^2}{\mathbf{1}^\top W_*^s(X)} - \omega_{n-1}. \tag{2.16}$$

Our aim is now to obtain a spherical analogue of Soto (2025, Thm. 4.3) by giving upper bounds on $e(X, W_*^s(X))^2$ and $e(X, W_0^s(X))^2$. To do so, we introduce the associated K_s-interpolant following the notation from Narcowich *et al.* (2007, Sec. 5), which is closely related to the estimator $\hat{V}_{W_*^s}$. For a function $f : S^{n-1} \to \mathbb{R}$, a K_s-interpolant of f on X is a function of the form

$$I_{X,K_s}(f) = \sum_{x \in X} c_x K(x, \cdot),$$

where the coefficient vector $c = (c_1, \dots, c_N)^\top$ satisfies $K_s(X)c = (f(x_1), \dots, f(x_N))^\top$. Assume from now on that the points in X are pairwise distinct. Then, as $K(X)$ is invertible, this interpolant is unique. For $\hat{V}_{W_*^s}(f; X)$, we have

$$\hat{V}_{W_*^s}(f; X) = \int_{S^{n-1}} I_{X,K_s}(f)(u)\, \mathscr{H}^{n-1}(du). \tag{2.17}$$

Indeed, the right hand side of (2.17) can be simplified using (2.9) to get

$$\int_{S^{n-1}} I_{X,K_s}(f)(u)\, \mathscr{H}^{n-1}(du) = \sum_{i=1}^N c_i,$$

which coincides with

$$\begin{aligned} \hat{V}_{W_*^s(X)}(f; X) &= W_*^s(X)^\top f_X \\ &= W_*^s(X)^\top K_s(X) c \\ &= 1^\top c = \sum_{i=1}^N c_i. \end{aligned}$$

This establishes the claim (2.17).

To state the deterministic error bound we define the following geometric quantities. Let $d_S(x, y)$ denote geodesic distance on S^{n-1}. For a finite set $X \subset S^{n-1}$, define the fill distance, separation radius, and mesh ratio by

$$h_X = \sup_{u \in S^{n-1}} \min_{x \in X} d_S(u, x), \quad q_X = \frac{1}{2} \min_{\substack{x,y \in X \\ x \neq y}} d_S(x, y),$$

$$\rho_X = \frac{h_X}{q_X}, \tag{2.18}$$

respectively. The quantity h_X measures coverage of the sphere, while q_X controls point separation. We can now state the spherical analogue of Soto (2025, Thm. 4.3). For $s' \geq s > (n-1)/2$, let $W_*^{s'}(X)$ and $W_0^{s'}(X)$ be the weights obtained from the smoother kernel $K_{s'}$. The new parameter s' controls the smoothness imposed through the choice of kernel, and may exceed the actual smoothness s of the integrand. This potential oversmoothing appears in the following theorem via the mesh ratio ρ_X, which disappears if $s' = s$.

In the proof of the following theorem Narcowich *et al.* (2007, Thm. 5.5) is crucial. This theorem is stated without any restriction on the fill distance h_X, although its proof relies on Narcowich *et al.* (2007, Prop. 5.3). This result is a restatement of Hubbert and Morton (2004, Thm. 3.4) in a specific case, which indeed requires that the fill distance h_X is sufficiently small.

This restriction can be removed. Indeed, if $h_X \geq h_0 > 0$ for some fixed h_0, then $1 \leq h_0^{-\tau} h_X^\tau$ for $\tau \geq n/2$, and the bound Narcowich *et al.* (2007, eq. (5.7)) follows using Narcowich *et al.* (2007, eq. (5.6)) to relate the norms involved. The resulting constant in the bound is then $C_1(h_0) = \sqrt{b} h_0^{-\tau}$, where b is a constant defined in relation to Narcowich *et al.* (2007, eq. (5.6)). Overall, one can derive Narcowich *et al.* (2007, eq. (5.7)) without any constraint on h_X by choosing h_0 sufficiently small and fixing the constant as the maximum of $C_1(h_0)$ and the one provided by Hubbert and Morton (2004, Thm. 3.4).

Related convergence results for spherical kernel quadrature were obtained by Fuselier *et al.* (2014, Thm. 4.10). Their analysis also relies on Narcowich *et al.* (2007, Thm. 5.5), as stated before their Proposition 4.3. Unlike their quadrature theorem, the following result retains the explicit dependence on the mesh ratio, allows real-valued smoothness parameters, and imposes no restriction on the fill distance h_X.

The case $s < s'$ corresponds to smoothness misspecification, which was also studied by Kanagawa *et al.* (2020, Thm. 2–3) for kernel-based quadrature on Euclidean domains.

Theorem 2.1. *Let $n \geq 2$ and $s' \geq s > (n-1)/2$. There exists a constant $C > 0$, depending only on n, s, s', such that for every finite set $X \subset S^{n-1}$ of at least two distinct points and every $f \in \mathbb{H}^s$,*

$$\left| I(f) - \widehat{V}_{W_*^{s'}}(f; X) \right| \leq C h_X^s \rho_X^{s'-s} \|f\|_{\mathbb{H}^s}. \tag{2.19}$$

Equivalently,

$$e_s(X, W_*^{s'}(X)) \leq C h_X^s \rho_X^{s'-s}.$$

Proof. Let $I_{X,K_{s'}}(f)$ denote the $K_{s'}$-interpolant of f on X,

$$I_{X,K_{s'}}(f) = \sum_{x\in X} c_x K_{s'}(x,\cdot), \qquad K_{s'}(X)c = f_X.$$

Using (2.17) with the kernel $K_{s'}$, we get

$$\begin{aligned}&\left|I(f) - \widehat{V}_{W_*^{s'}}(f;X)\right| \\ &= \left|\int_{S^{n-1}} \left(f - I_{X,K_{s'}} f\right)(u)\, \mathscr{H}^{n-1}(du)\right| \\ &\le \omega_{n-1}^{1/2} \left\|f - I_{X,K_{s'}} f\right\|_{L^2(S^{n-1})}.\end{aligned}$$

The interpolation estimate (Narcowich *et al.*, 2007, Thm. 5.5) now yields

$$\left\|f - I_{X,K_{s'}} f\right\|_{L^2(S^{n-1})} \le C h_X^s \rho_X^{s'-s} \|f\|_{\mathbb{H}^s}.$$

for some constant $C > 0$. Combining the two bounds gives (2.19). Taking the supremum over $\|f\|_{\mathbb{H}^s} \le 1$ gives the final statement. □

As a corollary, we have the following.

Corollary 2.2. *Under the assumptions of Theorem 2.1,*

$$e_s(X, W_0^{s'}(X)) \le C' h_X^s \rho_X^{s'-s},$$

where $C' > 0$ depends only on n, s, s'.

Proof. Let $X = \{x_1, \dots, x_N\} \subset S^{n-1}$. For $f \in \mathbb{H}^s$, define $f_0 = f - \frac{I(f)}{\omega_{n-1}}$. Using (2.14) and linearity, we get

$$\widehat{V}_{W_0^{s'}}(f;X) = c_X \widehat{V}_{W_*^{s'}}(f_0;X) + \widehat{V}_{W_0^{s'}}(I(f)/\omega_{n-1};X)$$

with $c_X = \frac{\omega_{n-1}}{\mathbf{1}^\top W_*^{s'}(X)}$.

As $(W_0^{s'})^\top \mathbf{1} = \omega_{n-1}$ the last term equals $I(f)$, and as $I(f_0) = 0$, we conclude

$$I(f) - \widehat{V}_{W_0^{s'}}(f;X) = c_X \left(I(f_0) - \widehat{V}_{W_*^{s'}}(f_0;X)\right). \quad (2.20)$$

As $\|f_0\|_{\mathbb{H}^s} \le \|f\|_{\mathbb{H}^s}$, we get $\{f_0 : \|f\|_{\mathbb{H}^s} \le 1\} \subseteq \{g : \|g\|_{\mathbb{H}^s} \le 1\}$. Consequently, using (2.20), we get

$$\begin{aligned}&e_s(X, W_0^{s'}(X)) \\ &\quad \le c_X \sup_{\|g\|_{\mathbb{H}^s}\le 1} \left|I(g) - \widehat{V}_{W_*^{s'}}(g;X)\right| \qquad (2.21) \\ &\quad = c_X e_s(X, W_*^{s'}(X)),\end{aligned}$$

so the proof is complete by Theorem 2.1 if we can bound $c_X = \omega_{n-1}/\mathbf{1}^\top W_*^{s'}(X)$ from above. To this end, define the inner product $\langle x,y\rangle_{K_{s'}} = x^\top K_{s'}(X) y$, for $x, y \in \mathbb{R}^N$. By Cauchy–Schwarz, we get

$$\begin{aligned}&\langle K_{s'}(X)^{-1}\mathbf{1}, \mathbf{1}\rangle_{K_{s'}}^2 \\ &\qquad \le \langle K_{s'}(X)^{-1}\mathbf{1}, K_{s'}(X)^{-1}\mathbf{1}\rangle_{K_{s'}} \cdot \langle \mathbf{1}, \mathbf{1}\rangle_{K_{s'}},\end{aligned}$$

or equivalently,

$$\mathbf{1}^\top W_*^{s'}(X) \ge \frac{N^2}{\mathbf{1}^\top K_{s'}(X)\mathbf{1}}.$$

As

$$\mathbf{1}^\top K_{s'}(X)\mathbf{1} = \sum_{x,y\in X} K_{s'}(x,y), \qquad (2.22)$$

we need a uniform bound on $K_{s'}$. For a reproducing kernel, which is invariant under simultaneous rotations of both arguments, Cauchy–Schwarz implies $|K_{s'}(x,y)| \le \|K_{s'}\|_\infty$ for any $x, y \in S^{n-1}$ with equality if $x = y$. From (2.22), we get

$$\mathbf{1}^\top K_{s'}(X)\mathbf{1} \le N^2 \|K_{s'}\|_\infty,$$

and we derive the lower bound $\mathbf{1}^\top W_*^{s'}(X) \ge 1/\|K_{s'}\|_\infty$. Inserting this in (2.21), the proof concludes after applying Theorem 2.1.

□

From (2.10), we now have a way to bound the integration error. If we choose $s = s'$ in Theorem 2.1, then the integration error tends to zero as the fill distance decreases. Thus, for a fixed sampling design X, one obtains deterministic error intervals whenever an upper bound on $\|f\|_{\mathbb{H}^s}$ is available.

STOCHASTIC IMPLICATIONS

We now turn to stochastic implications of the introduced theory. For simplicity, we focus on the rotational design $X_R = RX_0$ with $R \sim \nu$, where $X_0 \subset S^{n-1}$ is fixed.

If the weights are rotation covariant, elementary averaging over $SO(n)$ gives

$$\begin{aligned}\mathbb{E}_R \widehat{V}_w(f;X_R) &= \frac{S_w(X_0)}{\omega_{n-1}} I(f), \\ S_w(X_0) &= \sum_{x\in X_0} w(x, X_0).\end{aligned} \qquad (3.1)$$

In particular, the normalized weights W_0^s lead to an unbiased estimator, since $S_{W_0^s}(X_0) = \omega_{n-1}$. For the unconstrained optimal weights W_*^s, (2.15) gives the bias formula

$$\mathbb{E}_R \widehat{V}_{W_*^s}(f;X_R) = \left(1 - \frac{e_s(X_0, W_*^s(X_0))^2}{\omega_{n-1}}\right) I(f).$$

Hence, W_*^s is generally biased, but the bias is proportional to the squared worst-case error and tends to 0 for $h_X \to 0$ by Theorem 2.1.

The variance is controlled by the deterministic error bound. If we let

$$\bar{f} = \frac{I(f)}{\omega_{n-1}}, \qquad f_0 = f - \bar{f},$$

the constant part of f does not contribute to the variance. Therefore

$$\mathrm{Var}_R\Big(\widehat{V}_w(f;X_R)\Big) \le e_s(X_0, w(X_0))^2 \|f_0\|_{\mathbb{H}^s}^2.$$

Combining this with Theorem 2.1, we obtain, for $s' \ge s > (n-1)/2$,

$$\mathrm{Var}_R\Big(\widehat{V}_{W_*^{s'}}(f;X_R)\Big) \le C h_{X_0}^{2s} \rho_{X_0}^{2(s'-s)} \|f_0\|_{\mathbb{H}^s}^2,$$

and a similar bound holds for $W_0^{s'}$.

The remaining difficulty is that the full Sobolev norm $\|f\|_{\mathbb{H}^s}$ cannot be reliably estimated from finitely many point values without additional assumptions. Indeed, high-frequency spherical harmonics can vanish on the sampling points while having arbitrarily large Sobolev norm. As a possible approach to this problem let P_F be the orthogonal projection of a function in $L^2(S^{n-1})$ onto $\Pi_F = \bigoplus_{k=0}^F \mathbb{Y}_k^n$, and assume the tail condition

$$\|f - P_F f\|_{\mathbb{H}^s} \le \tau_F. \tag{3.2}$$

Then $\|f\|_{\mathbb{H}^s}^2 \le T_F(f) + \tau_F^2$ with

$$T_F(f) = \|P_F f\|_{\mathbb{H}^s}^2 = \sum_{k=0}^{F} (1+\lambda_k)^s \sum_{j=1}^{N_{k,n}} |\widehat{f}_{k,j}|^2,$$

and hence

$$\Big|I(f) - \widehat{V}_w(f;X_R)\Big| \le \big(T_F(f) + \tau_F^2\big)^{1/2} e_s(X_R, w). \tag{3.3}$$

To estimate $T_F(f)$, we propose the use of ordinary least squares. As this method is notationally heavy, further arguments and a proof of the theorem below are postponed until the end of the paper, and we only describe the core details here. For $F \in \mathbb{N}_0$, let $M_F = \dim \Pi_F = \sum_{k=0}^F N_{k,n}$. We define $A_F(X_R) \in \mathbb{R}^{N \times M_F}$ as the spherical harmonic design matrix up to degree F, given by

$$A_F(X) = \begin{pmatrix} Y_{0,1}(x_1) & Y_{1,1}(x_1) & \cdots & Y_{F,N_{F,n}}(x_1) \\ Y_{0,1}(x_2) & Y_{1,1}(x_2) & \cdots & Y_{F,N_{F,n}}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ Y_{0,1}(x_N) & Y_{1,1}(x_N) & \cdots & Y_{F,N_{F,n}}(x_N) \end{pmatrix}. \tag{3.4}$$

for $X = \{x_1, \dots, x_N\}$. Whenever $A_F(X_R)$ has full column rank, let

$$\widehat{c}_F^{\,\mathrm{LS}}(f;X_R) = \big(A_F(X_R)^\top A_F(X_R)\big)^{-1} A_F(X_R)^\top f_{X_R}. \tag{3.5}$$

and set

$$\widehat{T}_F^{\,\mathrm{LS}}(f;X_R) = \big(\widehat{c}_F^{\,\mathrm{LS}}(f;X_R)\big)^\top \Lambda_{F,s} \widehat{c}_F^{\,\mathrm{LS}}(f;X_R), \tag{3.6}$$

where $\Lambda_{F,s}$ is diagonal with entries $(1+\lambda_k)^s$, repeated according to the multiplicities $N_{k,n}$ for $0 \le k \le F$. For a matrix $A \in \mathbb{R}^{N \times m}$, define

$$\sigma_{\min}(A) = \inf_{\|u\|_2 = 1} \|Au\|_2 = \sqrt{\lambda_{\min}(A^\top A)}.$$

Thus A has full column rank precisely when $\sigma_{\min}(A) > 0$. In the following, $\sigma_{\min}(A_F(X_0))$ measures the stability of the least-squares reconstruction on Π_F.

Theorem 3.1 (Conservative 95% interval)**.** *Let $n \ge 2$, $s > (n-1)/2$, $F \in \mathbb{N}_0$, $f \in \mathbb{H}^s(S^{n-1})$, and $\tau_F \ge 0$. Let $X_R = RX_0$, where $X_0 \subset S^{n-1}$ is a fixed set of N points and $R \sim \nu$. Assume that $A_F(X_0)$ has full column rank (hence $N \ge M_F$) and that* (3.2) *holds. Then, with probability at least* 0.95*,*

$$\sqrt{T_F(f)} \le \sqrt{\widehat{T}_F^{\,\mathrm{LS}}(f;X_R)} + C_F(X_0)\tau_F,$$

where

$$C_F(X_0) = (1+\lambda_F)^{s/2} \sqrt{20\,\kappa_F(X_0)},$$
$$\kappa_F(X_0) = \frac{N}{\omega_{n-1}\sigma_{\min}(A_F(X_0))^2}.$$

Consequently, with probability at least 0.95*,*

$$I(f) \in \big[\widehat{V}_w(f;X_R) - R_{F,0.95}(X_R,w),\ \widehat{V}_w(f;X_R) + R_{F,0.95}(X_R,w)\big],$$

where

$$R_{F,0.95}(X_R,w) = \left(\left[\sqrt{\widehat{T}_F^{\,\mathrm{LS}}(f;X_R)} + C_F(X_0)\tau_F\right]^2 + \tau_F^2\right)^{1/2} \times e_s(X_R,w)$$

for any choice of quadrature weights $w = w(X_R) \in \mathbb{R}^N$.

We remark that this finite-sample randomization interval is deliberately conservative, as it is based on Markov's inequality and the deterministic tail bound (3.2). Since X_R is obtained by a single random rotation of a fixed design, standard central limit theorems for independent observations do not apply directly.

Nevertheless, this does not rule out the existence of an asymptotic distribution for a sequence of randomly rotated fixed designs.

Also, replacing the rotational design model with another stochastic point pattern on the sphere, it seems highly probable that better 95% confidence intervals could be achieved. For other stochastic processes, one can, for instance consider independent points on the sphere or determinantal point processes (see, for instance, Brauchart *et al.* (2020, p. 766)). Such underlying stochastic models may allow asymptotic distributional results, although proving a useful central limit theorem may require other assumptions, which may be explored in other works.
If one restricts to rotational designs, one could discuss how to choose X_0. To this end, we suggest letting X_0 be a *spherical t-design*, i.e, a finite set $X_0 \subset S^{n-1}$, for which the equal-weight quadrature rule is exact for all spherical polynomials of degree at most t. For more information on these types of designs, see Bondarenko *et al.* (2013); Delsarte *et al.* (1977). Tables of spherical designs can be found in Womersley (2018). As an example, the icosahedron with 12 vertices on S^2 is a spherical 5-design (Delsarte *et al.*, 1977, Example. 5.8).

Spherical t-designs also simplify the matrix $A_F(X_0)^\top A_F(X_0)$ based on (3.4) if t is sufficiently large. If X_0 is a spherical $2F$-design, then products of spherical harmonics of degree at most F are integrated exactly by the equal-weight rule. As a consequence, estimating $\widehat{c}_F^{\mathrm{LS}}(f;X_R)$ simplifies, as $A_F(X_0)^\top A_F(X_0)$ equals N/ω_{n-1} times the identity matrix, where N is the number of elements in X_0.

Indeed, if X_0 is a spherical $2F$-design given by $X_0 = \{x_1,\dots,x_N\}$, we denote the a'th column in $A_F(X_0)$ by $\tilde{Y}_a$ for $a = 1,\dots,M_F$. If the a-th column corresponds to the spherical harmonic $Y_{k,j}$, and the b-th column corresponds to $Y_{\ell,m}$ for some indices (k,j,ℓ,m), then

$$\begin{aligned} B_{ab} &= \Big(A_F(X_0)^\top A_F(X_0)\Big)_{ab} \\ &= \tilde{Y}_a^\top \tilde{Y}_b = \sum_{i=1}^{N} Y_{k,j}(x_i) Y_{\ell,m}(x_i). \end{aligned}$$

This is proportional to an equal weight rule for the function $Y_{k,j}(\cdot)Y_{\ell,m}(\cdot)$, we conclude that B_{ab} is proportional to the integral of this function over the sphere with proportionality constant N/ω_{n-1} as X_0 is a spherical $2F$-design. Using orthogonality arguments, we conclude that $B_{ab} = N/\omega_{n-1}$ if $a = b$ and zero otherwise giving the claim.

Another interesting direction is that of *hyperuniformity* on the sphere. The concept of hyperuniformity originates from Euclidean space, see for instance, Torquato and Stillinger (2003) for one of the first papers on the subject or the many references in Lotz and Klatt (2026). Hyperuniformity has recently been introduced on the sphere (Brauchart *et al.*, 2019; 2020; Lošdorfer Božič and Čopar, 2019; Meyra *et al.*, 2019). In the Euclidean setting, hyperuniformity is characterized by local density fluctuations of smaller order than for a Poisson point process, and the spherical analogues compare the cap number variance (Brauchart *et al.*, 2019). These ideas could be seen in relation to Monte Carlo designs as in Brauchart *et al.* (2014) and perhaps be extended into use for limit distributions.

We note that this approach is conceptually different from the approach taken in the present section. Here the point configuration X is treated as given, and the weights are adapted to that configuration. In a hyperuniform or QMC-design approach, one instead chooses the point configuration and typically uses equal weights. Thus, the present method may be viewed as fitting good weights to a fixed design, whereas QMC and hyperuniform methods aim to construct good designs for simple equal-weight quadrature.

As a final application of the theory developed so far, we consider an example from Stereology in dimension 2 and 3. Unlike the previous applications, this setting imposes stronger assumptions on the functions involved, and therefore no additional assumption on the norm of the tail is needed. Let $K \subset \mathbb{R}^n$ be a convex body with $o \in \operatorname{int} K$. In particular, K is non-empty and full-dimensional. We define the *radial function* of K by

$$\rho_K(u) = \sup\{r \geq 0 : ru \in K\}, \qquad u \in S^{n-1}.$$

Then, using Müller (1966, p. 1) it follows that the n-dimensional volume of K, $\lambda_n(K)$, is given by

$$\lambda_n(K) = \frac{1}{n} \int_{S^{n-1}} \rho_K(u)^n \, \mathscr{H}^{n-1}(du). \qquad (3.7)$$

This identity gives rise to so-called *nucleator* estimator, which has seen use in sampling applications, see Gundersen (1988); Vedel Jensen (1991) and references therein. We are now in position to bound the estimation error for the normalized weights and systematic random rotations.

To illustrate our approach, we consider the cases $n = 2$ and $n = 3$. For $n = 2$, there is a natural systematic design for every N, namely N equidistant points on S^1. For $n = 3$, no similar configuration exists for an arbitrary number N of points on S^2. The problem of distributing points uniformly on the sphere has therefore been studied see, for instance, the surveys Saff and Kuijlaars (1997); Brauchart and Grabner (2015). For a concrete illustration in dimension $n = 3$, we use the vertices of the regular icosahedron, which form a spherical 5-design on S^2.

We start with the case $n = 2$. We identify a function $f : S^1 \to \mathbb{C}$ with the 2π-periodic function

$$f(\theta) = f(\cos\theta, \sin\theta), \qquad \theta \in [0, 2\pi).$$

Under this identification, the spherical harmonics are the Fourier functions and the Laplace–Beltrami operator is the second derivative with respect to θ (Atkinson and Han, 2012, p. 90). Hence,

$$\|(-\Delta_{S^1})^{\ell/2} f\|^2_{L^2(S^1)} = \|f^{(\ell)}\|^2_{L^2([0,2\pi))},$$

where

$$f^{(\ell)}(\theta) = \sum_{k\in\mathbb{Z}} (ik)^\ell \widehat{f}(k) e^{ik\theta}$$

is the ℓth weak derivative, with the series converging in $L^2([0,2\pi))$. Therefore, by (2.6)

$$\|f\|^2_{\mathbb{H}^s(S^1)} = \sum_{\ell=0}^{s} \binom{s}{\ell} \|f^{(\ell)}\|^2_{L^2([0,2\pi))}, \quad f \in \mathbb{H}^s, \quad (3.8)$$

for $s \in \mathbb{N}$. Thus, the norm can be controlled by assuming uniform bounds on the norm of the derivatives of suitable order. One such example, that works for $s = 1$, is assuming

$$K \in \mathbb{K}(r,R) = \{K \subseteq \mathbb{R}^2 : K \text{ is convex and } rB^2 \subset K \subset RB^2\}$$

for some $0 < r < R < \infty$, where B^n is the unit ball in $\mathbb{R}^n$. We do not pursue the case $s > 1$ here, although the second part of the proof below extends directly once suitable bounds on higher-order weak derivatives are available.

Proposition 3.2. *Let $K \in \mathbb{K}(r,R)$ for $r < R$. Then*

$$\|\rho_K^2\|_{\mathbb{H}^1(S^1)} \le \sqrt{2\pi} R^2 \left(1 + 4\frac{R^2}{r^2}\right)^{1/2}.$$

Proof. If K° denotes the polar body of K, then $\rho_K = h_{K^\circ}^{-1}$ and $\frac{1}{R} \le h_{K^\circ}(\theta) \le \frac{1}{r}$ (Kiderlen, 2008, p. 2024). As $|h_{K^\circ}(\theta) - h_{K^\circ}(\eta)| \le \sup_{x\in K^\circ} \|x\| |\theta - \eta|$ for any $\theta, \eta \in [0, 2\pi)$, the previous upper bound implies that h_{K° is $1/r$-Lipschitz continuous, and by Rademacher's theorem, we get $|h'_{K^\circ}(\theta)| \le 1/r$ for almost all θ. These observations imply

$$\rho_K^2(\theta) = h_{K^\circ}^{-2}(\theta) \le R^2,$$
$$\left|(\rho_K^2)'(\theta)\right| = 2h_{K^\circ}^{-3}(\theta)\left|h'_{K^\circ}(\theta)\right| \le \frac{2R^3}{r}.$$

Consequently,

$$\|\rho_K^2\|^2_{L^2(S^1)} \le 2\pi R^4, \qquad \|(\rho_K^2)'\|^2_{L^2(S^1)} \le \frac{8\pi R^6}{r^2},$$

which implies the claim by (3.8). □

Accompanying this bound, we will now illustrate the asymptotic decay in Theorem 2.1 using the N-gon on S^1 for selected values of N. Let

$$X_0 = \{u_j : j = 0, \dots, N-1\} \subset S^1,$$
$$u_j = (\cos\theta_j, \sin\theta_j).$$

with $\theta_j = 2\pi j/N$. Since the kernel K_s is rotation invariant, the worst-case error is also rotation invariant, so it is enough to compute it for X_0. We remark that $h_{X_0} = \pi/N$, so we expect that $e_1(X_0, W_0^1) = O(N^{-1})$ for $N \to \infty$ due to Corollary 2.2. By (2.16) and the arguments before it, we get

$$W_0^s(X_0) = \frac{2\pi}{N}\mathbf{1},$$
$$e_s(X_0, W_0^s(X_0))^2 = \frac{(2\pi)^2}{N}\gamma_N - 2\pi,$$

where γ_N is the row-sum of $K_s(X_0)$. The kernel K_s on S^1 has the Fourier representation

$$K_s(\theta,\varphi) = \frac{1}{2\pi}\sum_{m\in\mathbb{Z}} (1+m^2)^{-s} e^{im(\theta-\varphi)},$$

for any two points on the unit circle given by the angle with the x-axis. In this notation, the row sums of the kernel matrix are

$$\gamma_N = \sum_{k=0}^{N-1} K_s(\theta_j, \theta_k)$$
$$= \frac{1}{2\pi}\sum_{m\in\mathbb{Z}} (1+m^2)^{-s} e^{im\theta_j} \sum_{k=0}^{N-1} e^{-im\theta_k}.$$

The inner sum vanishes unless $N \mid m$, in which case it equals N. Thus, we get

$$\gamma_N = \frac{N}{2\pi}\sum_{\ell\in\mathbb{Z}} (1+N^2\ell^2)^{-s},$$
$$e_s(X_0, W_0^s(X_0))^2 = 4\pi \sum_{\ell=1}^{\infty} (1+N^2\ell^2)^{-s}.$$

Combining this with (2.10) and Proposition 3.2, for every $K \in \mathbb{K}(r,R)$ and $s = 1$, this implies

$$\left|\lambda_2(K) - \frac{1}{2}\widehat{V}_{W_0^1}(\rho_K^2; X_R)\right|$$
$$\le \frac{\sqrt{2\pi}}{2} R^2 \left(1 + 4\frac{R^2}{r^2}\right)^{1/2}$$
$$\times \left[2\pi\left(\frac{\pi}{N}\coth\left(\frac{\pi}{N}\right) - 1\right)\right]^{1/2},$$

where the factor $\frac{1}{2}$ appears due to (3.7) and we simplified the infinite sum. A Taylor expansion gives $\left[2\pi\left(\frac{\pi}{N}\coth\left(\frac{\pi}{N}\right)-1\right)\right]^{1/2}$ decays at the expected rate N^{-1}. Moreover, as

$$\left[2\pi\left(\frac{\pi}{N}\coth\left(\frac{\pi}{N}\right)-1\right)\right]^{1/2}\approx\begin{cases}2.1161, & N=2,\\ 1.1143, & N=4,\\ 0.5654, & N=8,\\ 0.2839, & N=16,\\ 0.1420, & N=32,\end{cases}$$

the values displayed above indicate that the unspecified constants in Theorem 2.1 and Corollary 2.2 are of moderate size, so the asymptotic bounds appear useful even for relatively small values of N.

On S^2, the reproducing-kernel condition requires $s>1$, and the simplest integer choice is therefore $s=2$. By (2.6), control of first derivatives is not enough; one must also control the Laplace–Beltrami term. As in the example for $n=2$ the condition of convexity of K and $rB^3\subset K\subset RB^3$ provides a uniform bound on the first spherical derivatives of ρ_K, but not on its second derivatives. We therefore impose the additional assumption $\rho_K\in W^{2,\infty}(S^2)$, meaning that ρ_K has weak spherical derivatives up to order two which are essentially bounded. The constant L below gives a uniform bound on the second-order term $\Delta_{S^2}\rho_K$.

Proposition 3.3. *Let $K\subset\mathbb{R}^3$ be a convex body and let $0<r<R<\infty$. Suppose that*

$$rB^3\subset K\subset RB^3,$$
$$\rho_K\in W^{2,\infty}(S^2),\qquad \|\Delta_{S^2}\rho_K\|_\infty\le L.$$

Then $g_K=\rho_K^3\in\mathbb{H}^2(S^2)$, and

$$\|g_K\|^2_{\mathbb{H}^2(S^2)}\le 4\pi\left[R^6+\frac{18R^8}{r^2}+\left(3R^2L+\frac{6R^5}{r^2}\right)^2\right].$$

Proof. We use (2.6) with $s=2$ to get

$$\|g_K\|^2_{\mathbb{H}^2(S^2)}=\|g_K\|^2_{L^2(S^2)}+2\|(-\Delta_{S^2})^{1/2}g_K\|^2_{L^2(S^2)}+\|\Delta_{S^2}g_K\|^2_{L^2(S^2)}. \tag{3.9}$$

We now bound these terms in order of appearance. Using $r\le\rho_K\le R$, we obtain

$$\|g_K\|^2_{L^2(S^2)}\le 4\pi R^6.$$

For the second term, we use

$$\|(-\Delta_{S^2})^{1/2}g_K\|^2_{L^2(S^2)}=\|\nabla_{S^2}g_K\|^2_{L^2(S^2)},$$

which follows by self-adjointness of $(-\Delta_{S^2})^{1/2}$ and Atkinson and Han (2012, Prop. 3.3). To bound this, let $q=1/\rho_K$ be the support function of the polar body K°. Then

$$\nabla_{S^2}\rho_K=-\frac{\nabla_{S^2}q}{q^2}, \tag{3.10}$$

and $\nabla_{S^2}g_K=3\rho_K^2\nabla_{S^2}\rho_K$, by the chain rule. Thus, $|\nabla_{S^2}g_K|=3\rho_K^2|\nabla_{S^2}\rho_K|$ point-wise for almost all points in S^2.

We claim that $\|\nabla_{S^2}\rho_K\|_\infty\le R^2/r$. Indeed, since the function q is r^{-1}-Lipschitz on S^2, it satisfies $\|\nabla_{S^2}q\|_\infty\le r^{-1}$. Combining this with $R^{-1}B^3\subset K^\circ$ yields the claim by (3.10). In total,

$$\|\nabla_{S^2}g_K\|^2_{L^2(S^2)}\le 4\pi\left(3R^2\frac{R^2}{r}\right)^2=36\pi\frac{R^8}{r^2}.$$

For the last term in (3.9), the chain rule (see for instance, Atkinson and Han (2012, p. 91)) for the Laplace–Beltrami operator gives

$$\Delta_{S^2}g_K=3\rho_K^2\Delta_{S^2}\rho_K+6\rho_K|\nabla_{S^2}\rho_K|^2,$$

and the bound

$$\|\Delta_{S^2}g_K\|^2_{L^2(S^2)}\le 4\pi\left(3R^2L+6R\frac{R^4}{r^2}\right)^2=4\pi\left(3R^2L+\frac{6R^5}{r^2}\right)^2.$$

Combining the three upper bounds proves the claim. □

To illustrate how this bound can be applied, let $X_{\mathrm{ico}}\subset S^2$ be the set of the 12 vertices of a regular icosahedron. For X_{ico} there are exactly 4 different values of inner products between any two points in X_{ico}. Relative to any fixed vertex, the inner products with the vertices of the icosahedron are $1,-1,\frac{1}{\sqrt{5}},-\frac{1}{\sqrt{5}}$, where the last two values have multiplicity 5. By (2.8) the row sums of $K_s(X_{\mathrm{ico}})$ are constant and equal

$$\gamma_{\mathrm{ico},s}=\Phi_s(1)+\Phi_s(-1)+5\Phi_s\left(\frac{1}{\sqrt{5}}\right)+5\Phi_s\left(-\frac{1}{\sqrt{5}}\right).$$

Using (2.8) and the Legendre polynomial identities

$$P_{k,3}(1)=1,\qquad P_{k,3}(-t)=(-1)^kP_{k,3}(t),$$

we obtain

$$\gamma_{\mathrm{ico},s}=\sum_{\substack{k\ge0\\ k\text{ even}}}\big(1+k(k+1)\big)^{-s}\times\frac{2k+1}{4\pi}\left(2+10P_{k,3}\left(\frac{1}{\sqrt{5}}\right)\right). \tag{3.11}$$

By the arguments before (2.14), we thus get the two estimators

$$\frac{1}{3}\widehat{V}_{W_0^s}(g_K;X_R) = \frac{\pi}{9}\sum_{x\in X_R}\rho_K(x)^3, \tag{3.12}$$

$$\frac{1}{3}\widehat{V}_{W_*^s}(g_K;X_R) = \frac{1}{3\gamma_{\mathrm{ico},s}}\sum_{x\in X_R}\rho_K(x)^3. \tag{3.13}$$

for estimating the volume $\lambda_3(K)$. To bound the error, we let $E_{0,s}$ and $E_{*,s}$, denote the worst-case error squared for the two weights W_0^s and W_*^s, respectively. Focusing on $E_{0,s}$ the formulas (2.16) and (3.11) gives

$$E_{0,s} = \frac{\pi}{3}\sum_{\substack{k\geq 1\\ k \text{ even}}}(2k+1)\left(2+10P_{k,3}\left(\frac{1}{\sqrt{5}}\right)\right) \times \big(1+k(k+1)\big)^{-s},$$

where the term corresponding to $k=0$ cancels. Recall that X_{ico} is a spherical 5-design (Delsarte *et al.* (1977)), so the terms in $E_{0,s}$ corresponding to $k=2$ and $k=4$ also vanish. As $P_{8,3}\left(\frac{1}{\sqrt{5}}\right) = -\frac{1}{5}$, the term corresponding to $k=8$ also vanishes. Calculating the first 3 non-zero terms in $E_{0,s}$, we get

$$E_{0,s} = \frac{572\pi}{25}43^{-s} + \frac{6916\pi}{625}111^{-s} + O(157^{-s}), \qquad s\to\infty.$$

For $s=2$, numerical calculations give $E_{0,2}\approx 0.05073216$ and $E_{*,2}\approx 0.05052817$, so we can get a bound on the integration error by (2.10). If we furthermore assume that K satisfies the assumptions in Proposition 3.3, then

$$\left|\frac{1}{3}\widehat{V}_{W_0^2}(g_K;X_R)-\lambda_3(K)\right| \leq \frac{\sqrt{E_{0,2}}}{3}C_{r,R,L}\approx 0.0750793\,C_{r,R,L},$$

$$\left|\frac{1}{3}\widehat{V}_{W_*^2}(g_K;X_R)-\lambda_3(K)\right| \leq \frac{\sqrt{E_{*,2}}}{3}C_{r,R,L}\approx 0.0749282\,C_{r,R,L}.$$

with

$$C_{r,R,L} = \sqrt{4\pi}\left[R^6+\frac{18R^8}{r^2}+\left(3R^2L+\frac{6R^5}{r^2}\right)^2\right]^{1/2}.$$

Thus, even though only $N=12$, the contribution from the icosahedral quadrature design is relatively small. Moreover, the improvement obtained from the unconstrained weights W_*^2 is negligible as the two constants differ by approximately 0.2%. This suggests that W_0^2 is the more natural choice in this case.

The bounds remain conservative, since $C_{r,R,L}$ may be large when R/r or L is large, and their derivation uses several uniform inequalities. Their main advantage is therefore an explicit error guarantee that holds uniformly over the stated class of convex bodies. A small refinement is available because X_{ico} is a spherical 5-design. We can use the orthogonal projection onto the spherical harmonics of degree at most 5, P_5 to get,

$$I(g_K)-\widehat{V}_{W_0^2}(g_K;X_R) = I(g_K-P_5g_K)-\widehat{V}_{W_0^2}(g_K-P_5g_K;X_R).$$

Consequently,

$$\left|\frac{1}{3}\widehat{V}_{W_0^2}(g_K;X_R)-\lambda_3(K)\right| \leq \frac{\sqrt{E_{0,2}}}{3}\|g_K-P_5g_K\|_{\mathbb{H}^2(S^2)}.$$

This removes all low-frequency components of degree at most 5 and can be sharper than the bound involving the full Sobolev norm.

Further improvements are possible under stronger regularity assumptions of the type used in Proposition 3.3. If sufficiently many spherical derivatives of ρ_K admit uniform bounds, one may work in $\mathbb{H}^s(S^2)$ for $s>2$. The same 5-design argument then gives

$$\left|\frac{1}{3}\widehat{V}_{W_0^s}(g_K;X_R)-\lambda_3(K)\right| \leq \frac{\sqrt{E_{0,s}}}{3}\|g_K-P_5g_K\|_{\mathbb{H}^s(S^2)}.$$

Since $E_{0,s}$ decreases rapidly with s, this may yield substantially smaller bounds for sufficiently smooth bodies, provided that the corresponding higher-order Sobolev norm can be controlled. With this observation, we end the paper with the postponed proof of Theorem 3.1.

Proof of Theorem 3.1. Let the notation be as introduced before Theorem 3.1. The proof is based on comparing the least-squares coefficients given in (3.5) with the coefficients of $P_F f$. The main idea in the proof is to compare $T_F(f)$ to $\widehat{T}_F^{\mathrm{LS}}(f;X_R)$, defined in (3.6), and applying (3.3). To simplify the notation, let

$$c = c_F(f), \qquad \widehat{c} = \widehat{c}_F^{\mathrm{LS}}(f;X_R), \qquad \delta_R = \widehat{c}-c.$$

Then

$$T_F(f) = c^\top\Lambda_{F,s}c, \qquad \widehat{T}_F^{\mathrm{LS}}(f;X_R) = \widehat{c}^\top\Lambda_{F,s}\widehat{c}.$$

Since $c=\widehat{c}-\delta_R$, we get

$$T_F(f) = \|\Lambda_{F,s}^{1/2}(\widehat{c}-\delta_R)\|_2^2,$$

which can be seen by expanding both sides of the equation. Using the triangle inequality, we get

$$\sqrt{T_F(f)} \leq \|\Lambda_{F,s}^{1/2}\widehat{c}\|_2 + \|\Lambda_{F,s}^{1/2}\delta_R\|_2$$

and the upper bound

$$T_F(f) \leq \left(\sqrt{\widehat{T}_F^{\mathrm{LS}}(f;X_R)} + \eta_R\right)^2, \tag{3.14}$$

with

$$\eta_R = \|\Lambda_{F,s}^{1/2}\delta_R\|_2.$$

It remains to prove that η_R is small with high probability. We have the Cauchy–Schwarz upper bound on η_R

$$\eta_R^2 \leq (1+\lambda_F)^s \|\delta_R\|_2^2 \tag{3.15}$$

as

$$\|\Lambda_{F,s}^{1/2}\|_{\mathrm{op}} = (1+\lambda_F)^{s/2},$$

where $\|A\|_{op} = \sup_{u\in S^{m-1}} \|Au\|_2$ for $A \in \mathbb{R}^{n\times m}$. We will now give a bound on $\|\delta_R\|_2^2$. Let $r_F = f - P_F f$. Then by linearity, we get

$$\delta_R = \widehat{c} - c = \left(A_F(X_R)^\top A_F(X_R)\right)^{-1} A_F(X_R)^\top r_F(X_R).$$

and

$$\begin{aligned}
&\|\delta_R\|_2 \\
&= \left\| \left(A_F(X_R)^\top A_F(X_R)\right)^{-1} A_F(X_R)^\top r_F(X_R) \right\|_2 \\
&\leq \left\| \left(A_F(X_R)^\top A_F(X_R)\right)^{-1} A_F(X_R)^\top \right\|_{\mathrm{op}} \|r_F(X_R)\|_2
\end{aligned} \tag{3.16}$$

We now claim that

$$\left\| \left(A_F(X_R)^\top A_F(X_R)\right)^{-1} A_F(X_R)^\top \right\|_{\mathrm{op}} = \frac{1}{\sigma_{\min}(A_F(X_R))}. \tag{3.17}$$

To show this, we let

$$B = \left(A_F(X_R)^\top A_F(X_R)\right)^{-1} A_F(X_R)^\top.$$

Then $\|B\|_{op}^2$ equals the maximal eigenvalue of $BB^\top$. As the maximal eigenvalue of $BB^\top$ corresponds to the reciprocal of the minimal eigenvalue of $(BB^\top)^{-1}$ the claim (3.17) follows by expanding $(BB^\top)^{-1}$ and using the definition of $\sigma_{\min}$. Applying (3.17) to (3.16), we get

$$\|\delta_R\|_2^2 \leq \frac{1}{\sigma_{\min}(A_F(X_R))^2} \|r_F(X_R)\|_2^2.$$

The action of R on Π_F is represented by an orthogonal matrix $D_F(R)$, so $A_F(X_R) = A_F(X_0)D_F(R)$. Hence $\sigma_{\min}(A_F(RX_0)) = \sigma_{\min}(A_F(X_0))$, and by (3.15), we get

$$\mathbb{E}[\eta_R^2] \leq \frac{(1+\lambda_F)^s}{\sigma_{\min}(A_F(X_0))^2} \mathbb{E}\|r_F(X_R)\|_2^2. \tag{3.18}$$

It remains to compute the last expectation. Since each point in X_R is uniformly distributed on S^{n-1} linearity of the mean gives

$$\begin{aligned}
\mathbb{E}\|r_F(X_R)\|_2^2 &= \sum_{x\in X_0} \mathbb{E}\left[r_F(Rx)^2\right] \\
&= \frac{N}{\omega_{n-1}} \|r_F\|_{L^2(S^{n-1})}^2 \\
&\leq \frac{N}{\omega_{n-1}} \tau_F^2.
\end{aligned} \tag{3.19}$$

using the tail assumption in the last inequality. The rest of the proof is a use of Markov's inequality. Letting $C_F(X_0)$ and $\kappa_F(X_0)$ be given as in Theorem 3.1 Markov's inequality implies

$$\mathbb{P}_R\left(\eta_R > C_F(X_0)\tau_F\right) \leq 0.05.$$

after combining the two bounds (3.18) and (3.19). Thus, with probability at least 0.95,

$$\eta_R \leq C_F(X_0)\tau_F.$$

Combining this with (3.14), we get

$$T_F(f) \leq \left(\sqrt{\widehat{T}_F^{\mathrm{LS}}(f;X_R)} + C_F(X_0)\tau_F\right)^2.$$

Finally, inserting this into the deterministic error bound yields, with probability at least 0.95,

$$\begin{aligned}
&\left|I(f) - \widehat{V}_w(f;X_R)\right| \\
&\leq \left[\left(\sqrt{\widehat{T}_F^{\mathrm{LS}}(f;X_R)} + C_F(X_0)\tau_F\right)^2 + \tau_F^2\right]^{1/2} \\
&\qquad \times e_s(X_R, w).
\end{aligned}$$

This proves the claim. □

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DATA AVAILABILITY

No new data were generated or analyzed in this study.

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