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On the Koksma–Hlawka inequality

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The classical Koksma–Hlawka inequality does not apply to functions with simple discontinuities. Here we state a Koksma–Hlawka type inequality which applies to piecewise smooth functions $f\chi_\Omega$, with f smooth and Ω a Borel subset of $[0,1]^d$:

$$\left|N^{-1}\sum_{j=1}^{N}(f\chi_\Omega)(x_j)-\int_\Omega f(x)dx\right|\le \mathcal{D}\left(\Omega,\{x_j\}_{j=1}^N\right)\mathcal{V}(f),$$

where $\mathcal{D}\left(\Omega,\{x_j\}_{j=1}^N\right)$ is the discrepancy

$$\mathcal{D}\left(\Omega,\{x_j\}_{j=1}^N\right)=2^d\sup_{I\subseteq[0,1]^d}\left\{\left|N^{-1}\sum_{j=1}^{N}\chi_{\Omega\cap I}(x_j)-|\Omega\cap I|\right|\right\},$$

the supremum is over all d-dimensional intervals, and $\mathcal{V}(f)$ is the total variation

$$\mathcal{V}(f)=\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\int_{[0,1]^d}\left|\left(\frac{\partial}{\partial x}\right)^\alpha f(x)\right|dx.$$

We state similar results with variation and discrepancy measured by L^p and L^q norms, $1/p+1/q=1$, and we also give extensions to compact manifolds.

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1. Introduction

Koksma's inequality is a neat bound for the error in a numerical integration:

$$\left| N^{-1} \sum_{j=1}^{N} f\left(x_j\right) - \int_0^1 f(x)dx \right| \leq \mathcal{D}\left(\left\{x_j\right\}_{j=1}^{N}\right) \mathcal{V}(f).$$

In this inequality $\mathcal{D}\left(\left\{x_j\right\}_{j=1}^{N}\right)$ is the discrepancy of the points $0 \leq x_j \leq 1$ and $\mathcal{V}(f)$ is the total variation of the function f,

$$\mathcal{D}\left(\left\{x_j\right\}_{j=1}^{N}\right) = \sup_{0\leq t\leq 1} \left\{ \left| N^{-1} \sum_{j=1}^{N} \chi_{[0,t]}\left(x_j\right) - t \right| \right\},$$

$$\mathcal{V}(f) = \sup_{0=y_0<y_1<y_2<\cdots<y_n=1} \left\{ \sum_{k=1}^{n} |f\left(y_k\right) - f\left(y_{k-1}\right)| \right\}.$$

See [9]. We may say that Koksma's inequality is a simple machine which turns the discrepancy for a small family of functions, characteristic functions of intervals, into the discrepancy for a larger family, functions of bounded variation. The extension to several variables is a more delicate problem, yet it is of some relevance in numerical analysis. See e.g. [7–9,11,12,16]. A classical approach starts with the definitions of Vitali and Hardy–Krause variations. A partition of $[0, 1]^d$ is a set of d finite sequences $0 = \eta(k, 0) < \eta(k, 1) < \cdots < \eta(k, n_k) = 1$, with $k = 1, 2, \ldots, d$, and this partition splits $[0, 1]^d$ into d-dimensional intervals which are products of the 1-dimensional intervals $[\eta(k, j), \eta(k, j+1)]$. For a function f on $[0, 1]^d$ and for every d-dimensional interval I in $[0, 1]^d$ with edges parallel to the axes, let $\Delta(f, I)$ be an alternating sum of the values of f at the vertices of I. The Vitali variation is

$$V(f) = \sup_{R} \left\{ \sum_{I\in R} |\Delta(f, I)| \right\},$$

where the supremum is over all finite partitions R of $[0, 1]^d$. The Hardy–Krause variation is

$$\mathcal{V}(f) = \sum_{k} V_k(f),$$

where the sum is over the Vitali variations $V_k(f)$ of the restrictions of f to all faces anchored at $(1, 1, \ldots, 1)$. The discrepancy of a finite point set $\left\{x_j\right\}_{j=1}^{N}$ in $[0, 1]^d$ is defined by

$$\mathcal{D}\left(\left\{x_j\right\}_{j=1}^{N}\right) = \sup_{I} \left\{ \left| N^{-1} \sum_{j=1}^{N} \chi_I\left(x_j\right) - |I| \right| \right\},$$

where I is an interval of the form $[0, t_1] \times [0, t_2] \times \cdots \times [0, t_d]$ with $0 \leq t_k \leq 1$, and $|I| = t_1 t_2 \ldots t_d$ is its measure. The classical Koksma–Hlawka inequality states that if f has bounded Hardy–Krause variation, then

$$\left| N^{-1} \sum_{j=1}^{N} f\left(x_j\right) - \int_{[0,1]^d} f(x)dx \right| \leq \mathcal{D}\left(\left\{x_j\right\}_{j=1}^{N}\right) \mathcal{V}(f).$$

See [9, 2.5], [11, 1.4], [12, 2.2]. The assumptions required in the 1-dimensional Koksma inequality are satisfied by many familiar functions and are usually easy to verify. On the contrary, the Hardy–Krause condition in the Koksma–Hlawka inequality seems to be rather strict. It works well for smooth functions, but it cannot be applied to most functions with simple discontinuities. For example, the characteristic function of a convex polyhedron has bounded Hardy–Krause variation only if the polyhedron is a d-dimensional interval. For this and other reasons, several variants of the Koksma–Hlawka inequality have been proposed. In particular, in [6] the small family consists of characteristic functions of convex sets and the large family is given by functions with super level sets which are differences of finite unions of convex sets. See also [5,11,15, p. 162]. Finally, a general and systematic approach to Koksma–Hlawka inequalities is via reproducing kernel Hilbert spaces. See e.g. [1,7]. However, in some of these approaches the geometric meaning of the discrepancy is somehow hidden. The aim of this paper is to state Koksma–Hlawka inequalities with explicit geometric discrepancies, which apply to piecewise smooth functions, that is, smooth functions f restricted to arbitrary Borel sets Ω. In one of these inequalities, Theorem 1, the error in the numerical integration of $f\chi_\Omega$ is controlled by a variation of f defined in terms of derivatives, times the discrepancy of the intersection of Ω with translates of intervals I with edges parallel to the axes. In another version, Theorem 7, the discrepancy is with respect to the intersection of Ω with cubes, and in a further version, Theorem 9, the discrepancy is with respect to the intersection of Ω with balls. These results are first stated and proved when the underlying space is a torus, then they are extended to compact manifolds, Theorem 10, and, in particular, spheres, Theorem 13.

2. Koksma–Hlawka inequalities on a torus

In what follows we consider functions f, measures μ, and distributions on the torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d = [0, 1)^d$, that is, functions, measures, and distributions on $\mathbb{R}^d$ which are $\mathbb{Z}^d$ periodic, and Borel sets Ω in $\mathbb{R}^d$, not necessarily periodic.

Theorem 1. *If f is a continuous function on $\mathbb{T}^d$, if μ is a finite complex valued Borel measure on $\mathbb{T}^d$, if Ω is a bounded Borel subset of $\mathbb{R}^d$, and if $1 \le p, q \le +\infty$ with $1/p + 1/q = 1$, then*

$$\left| \int_\Omega f(x)\overline{d\mu(x)} \right| \le \mathcal{D}_q(\Omega, \mu)\, \mathcal{V}_p(f),$$

where $\mathcal{D}_q(\Omega, \mu)$ is the L^q discrepancy

$$\mathcal{D}_q(\Omega, \mu) = \int_{[0,1]^d} \left\{ \int_{\mathbb{T}^d} \left| \sum_{n\in\mathbb{Z}^d} \mu\left((x + n - I(t)) \cap \Omega\right) \right|^q dx \right\}^{1/q} dt,$$

with $t = (t_1, \ldots, t_d)$, $0 \le t_k \le 1$, $I(t) = [0, t_1] \times \cdots \times [0, t_d]$, $x + n - I(t)$ is the set of all points y with $x + n - y$ in $I(t)$, and $\mathcal{V}_p(f)$ is the L^p total variation

$$\mathcal{V}_p(f) = \sum_{\alpha\in\{0,1\}^d} 2^{d-|\alpha|} \left\{ \int_{\mathbb{T}^d} \left| \left(\frac{\partial}{\partial x}\right)^\alpha f(x) \right|^p dx \right\}^{1/p},$$

where the sum is over all the multiindices α which take only the values 0 and 1, $|\alpha|$ is the number of 1's, and $(\partial/\partial x)^\alpha = (\partial/\partial x_1)^{\alpha_1} \ldots (\partial/\partial x_d)^{\alpha_d}$.

The assumption $\mathcal{V}_p(f) < +\infty$ already implies that f is almost everywhere equal to a continuous function. Since the measure μ may have a singular part, it is necessary to fix a representative for f, and the canonical choice is the continuous representative. When $p = 1$ the theorem holds also when $(\partial/\partial x)^\alpha f(x)$ are finite measures, with $\int_{\mathbb{T}^d} |(\partial/\partial x)^\alpha f(x)|\, dx$ replaced by the total mass of these measures, but in this case the continuity of the function is not automatic and it has to be assumed. Also observe that less than d integrable derivatives are not enough to guarantee the boundedness and continuity of the function. Hence, if the measure μ is concentrated on the singularities of the function f, then the integral $\int_\Omega f(x)d\mu(x)$ may be not defined. The variation $\mathcal{V}_p(f)$ decreases with p, but if p decreases then q increases, and the discrepancy $\mathcal{D}_q(\Omega, \mu)$ increases. Hence a gain in p corresponds to a loss in q, and the optimal choice of these indices is the one that minimizes the product $\mathcal{D}_q(\Omega, \mu)\, \mathcal{V}_p(f)$. When Ω is contained in $[0, 1]^d$, the L^∞ discrepancy is dominated as follows:

$$\mathcal{D}_\infty(\Omega, \mu) \le 2^d \sup_{I\subseteq[0,1]^d} \left\{ |\mu(I \cap \Omega)| \right\}.$$

This reflects the difference between the discrepancy in a torus and the one in a cube, and it is due to the fact that an interval in $\mathbb{T}^d$ can be split into at most 2^d intervals in $[0, 1]^d$. In the classical Koksma–Hlawka inequality, and in most of discrepancy theory, the measure μ is the difference between masses δ_{x_j} concentrated at some points x_j and the uniformly distributed measure dx:

$$d\mu = N^{-1} \sum_{j=1}^{N} \delta_{x_j} - dx.$$

For this measure and when $p = 1$ and $\Omega = [0, 1]^d$ the above theorem is essentially equivalent to the classical Koksma–Hlawka inequality with respect to the Hardy–Krause variation. The proof of the theorem can be split into a sequence of easy lemmas. The first one is a Fourier analog of a multidimensional integration by parts in [16]. See also the examples in [1]. In what follows $\widehat{f}(n) = \int_{\mathbb{T}^d} f(x)e^{-2\pi i n\cdot x}dx$ denotes the Fourier transform and $g * \mu(x) = \int_{\mathbb{T}^d} g(x-y)d\mu(y)$ the convolution, and these operators are applied also to distributions.

Lemma 2. *Let φ be a non vanishing complex sequence on $\mathbb{Z}^d$, and assume that both φ and $1/\varphi$ have tempered growth in $\mathbb{Z}^d$. Also let f be a smooth function on $\mathbb{T}^d$. Define*

$$g(x) = \sum_{n\in\mathbb{Z}^d} \overline{\varphi(n)^{-1}} e^{2\pi i n\cdot x},$$
$$\mathfrak{D}f(x) = \sum_{n\in\mathbb{Z}^d} \varphi(n)\widehat{f}(n)e^{2\pi i n\cdot x}.$$

Finally, let μ be a finite measure on $\mathbb{T}^d$. Then the following identity holds:

$$\int_{\mathbb{T}^d} f(x)\overline{d\mu(x)} = \int_{\mathbb{T}^d} \mathfrak{D}f(x)\overline{g * \mu(x)}dx.$$

Proof. The assumptions on the growth of φ and $1/\varphi$ guarantee that $\mathfrak{D}f$ is a smooth function and g is a tempered distribution. Moreover

$$\begin{aligned}\int_{\mathbb{T}^d} f(x)\overline{d\mu(x)} &= \sum_{n\in\mathbb{Z}^d} \widehat{f}(n)\overline{\widehat{\mu}(n)} \\ &= \sum_{n\in\mathbb{Z}^d} \left(\varphi(n)\widehat{f}(n)\right)\left(\varphi(n)^{-1}\overline{\widehat{\mu}(n)}\right) = \int_{\mathbb{T}^d} \mathfrak{D}f(x)\overline{g * \mu(x)}dx. \quad \square\end{aligned}$$

Suitable choices of φ and μ will make the above abstract lemma more explicit and interesting. In particular, φ will be the Fourier transform of a differential integral operator and $1/\varphi$ the Fourier transform of a superposition of characteristic functions.

Lemma 3. *Let the function h on $\mathbb{R}^d$ be the superposition of the characteristic functions of all intervals $I(t) = [0, t_1] \times \cdots \times [0, t_d]$ with $0 \le t_k \le 1$, and let $g(x)$ be the $\mathbb{Z}^d$ periodization of h,*

$$h(x) = \int_{[0,1]^d} \chi_{I(t)}(x)dt, \qquad g(x) = \sum_{n\in\mathbb{Z}^d} h(x+n).$$

Then the function g has Fourier expansion

$$g(x) = \sum_{n\in\mathbb{Z}^d} \left(\prod_{k=1}^{d} (2\delta(n_k) + 2\pi i n_k)^{-1}\right) e^{2\pi i n\cdot x},$$

where $n = (n_1, \ldots, n_d)$, $\delta(n_k) = 1$ if $n_k = 0$ and $\delta(n_k) = 0$ if $n_k \neq 0$.

Proof. Observe that if $x = (x_1, \ldots, x_d)$, then

$$h(x) = \prod_{k=1}^{d} \int_0^1 \chi_{[0,t_k]}(x_k)\, dt_k = \prod_{k=1}^{d} (1 - x_k)\, \chi_{[0,1]}(x_k).$$

Now compute the Fourier coefficients,

$$\begin{aligned}\widehat{g}(n) &= \int_{\mathbb{T}^d} g(x) e^{-2\pi i n \cdot x} dx \\ &= \prod_{k=1}^{d} \left(\int_0^1 (1 - x_k)\, e^{-2\pi i n_k x_k} dx_k \right) = \prod_{k=1}^{d} (2\delta(n_k) + 2\pi i n_k)^{-1}. \quad \square\end{aligned}$$

Lemma 4. *If f is a smooth function on $\mathbb{T}^d$, then*

$$\begin{aligned}\mathfrak{D}f(x) &= \sum_{n \in \mathbb{Z}^d} \left(\prod_{k=1}^{d} (2\delta(n_k) - 2\pi i n_k) \right) \widehat{f}(n)\, e^{2\pi i n x} \\ &= \sum_{\alpha, \beta \in \{0,1\}^d,\ \alpha+\beta=(1,\ldots,1)} (-1)^{|\alpha|}\, 2^{|\beta|} \int_{[0,1]^{|\beta|}} \left(\frac{\partial}{\partial x} \right)^{\alpha} f\left(x + y^{\beta}\right) dy^{\beta}.\end{aligned}$$

We are using the notation $(\partial/\partial x)^{\alpha} = (\partial/\partial x_1)^{\alpha_1} \ldots (\partial/\partial x_d)^{\alpha_d}$ and $y^{\beta} = \sum_{j=1}^{d} \beta_j y_j e_j$, where $\left\{e_j\right\}_{j=1}^{d}$ is the canonical basis of $\mathbb{R}^d$, and $dy^{\beta} = dy_1^{\beta_1} \ldots dy_d^{\beta_d}$.

Proof. For any $\alpha \in \{0,1\}^d$ let

$$Z_{\alpha} = \left\{ n \in \mathbb{Z}^d : n_j = 0 \text{ if } \alpha_j = 0 \text{ and } n_j \neq 0 \text{ if } \alpha_j = 1 \right\}.$$

Since $\{Z_{\alpha}\}_{\alpha \in \{0,1\}^d}$ is a partition of $\mathbb{Z}^d$ we have

$$\begin{aligned}\mathfrak{D}f(x) &= \sum_{\alpha \in \{0,1\}^d} \sum_{n \in Z_{\alpha}} \left(\prod_{k=1}^{d} (2\delta(n_k) - 2\pi i n_k) \right) \widehat{f}(n) e^{2\pi i n x} \\ &= \sum_{\alpha \in \{0,1\}^d} \sum_{n \in Z_{\alpha}} 2^{d-|\alpha|} (-1)^{|\alpha|} \left(\prod_{k=1,\ldots,d \text{ and } \alpha_k=1} (2\pi i n_k) \right) \widehat{f}(n) e^{2\pi i n x}.\end{aligned}$$

For a fixed $\alpha \in \{0,1\}^d$ let $\beta \in \{0,1\}^d$ such that $\alpha + \beta = (1, \ldots, 1)$ and let

$$g_{\beta}(x) = \int_{[0,1]^{|\beta|}} \left(\frac{\partial}{\partial x} \right)^{\alpha} f\left(x + y^{\beta}\right) dy^{\beta}.$$

A simple computation shows that when $n \notin Z_{\alpha}$ then $\widehat{g_{\beta}}(n) = 0$, while when $n \in Z_{\alpha}$ then

$$\widehat{g_{\beta}}(n) = \left(\prod_{k=1,\ldots,d \text{ and } \alpha_k=1} (2\pi i n_k) \right) \widehat{f}(n).$$

Therefore

$$\mathfrak{D}f(x) = \sum_{\alpha, \beta \in \{0,1\}^d,\ \alpha+\beta=(1,\ldots,1)} (-1)^{|\alpha|}\, 2^{|\beta|} \int_{[0,1]^{|\beta|}} \left(\frac{\partial}{\partial x} \right)^{\alpha} f\left(x + y^{\beta}\right) dy^{\beta}. \quad \square$$

Proof of Theorem 1. By a limit argument, one can assume that f is smooth. Otherwise, it suffices to consider a sequence of smooth functions $\{f_n\}$, with

$$\lim_{n\to+\infty}\left\{\int_{\mathbb{T}^d}|f_n(x)-f(x)|\,d|\mu|(x)\right\}=0,$$

$$\lim_{n\to+\infty}\left\{\int_{\mathbb{T}^d}\left|\left(\frac{\partial}{\partial x}\right)^{\alpha}(f_n(x)-f(x))\right|^p dx\right\}^{1/p}=0.$$

We have to integrate a periodic smooth function f against a periodic measure μ over an arbitrary non periodic Borel set Ω in $\mathbb{R}^d$. By Lemma 2 applied to the periodization ν of the measure $\chi_\Omega\mu$, and by Hölder inequality, with g and $\mathfrak{D}f$ defined as in Lemmas 3 and 4 respectively,

$$\begin{aligned}\left|\int_\Omega f(x)\overline{d\mu(x)}\right| &= \left|\int_{\mathbb{T}^d} f(x)\left(\sum_{n\in\mathbb{Z}^d}\chi_\Omega(x+n)\right)\overline{d\mu(x)}\right| \\ &= \left|\int_{\mathbb{T}^d} f(x)\overline{d\nu(x)}\right| \le \|\mathfrak{D}f\|_{L^p(\mathbb{T}^d)}\,\|g*\nu\|_{L^q(\mathbb{T}^d)}\,.\end{aligned}$$

The estimate for $\|\mathfrak{D}f\|_{L^p(\mathbb{T}^d)}$ follows from Lemma 4,

$$\left\{\int_{\mathbb{T}^d}|\mathfrak{D}f(x)|^p\,dx\right\}^{1/p}\le\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\left\{\int_{\mathbb{T}^d}\left|\left(\frac{\partial}{\partial x}\right)^{\alpha}f(x)\right|^p dx\right\}^{1/p}.$$

The estimate for $\|g*\nu\|_{L^q(\mathbb{T}^d)}$ follows from Lemma 3,

$$\begin{aligned}&\left\{\int_{\mathbb{T}^d}|g*\nu(x)|^q\,dx\right\}^{1/q}\\ &=\left\{\int_{\mathbb{T}^d}\left|\int_{\mathbb{T}^d}\left(\sum_{m\in\mathbb{Z}^d}\int_{[0,1]^d}\chi_{I(t)}(x-y+m)\,dt\right)\left(\sum_{n\in\mathbb{Z}^d}\chi_\Omega(y+n)\right)d\mu(y)\right|^q dx\right\}^{1/q}\\ &=\left\{\int_{\mathbb{T}^d}\left|\int_{[0,1]^d}\left(\sum_{n\in\mathbb{Z}^d}\int_{\mathbb{R}^d}\chi_{I(t)}(x+n-z)\,\chi_\Omega(z)d\mu(z)\right)dt\right|^q dx\right\}^{1/q}\\ &=\left\{\int_{\mathbb{T}^d}\left|\int_{[0,1]^d}\left(\sum_{n\in\mathbb{Z}^d}\mu\left((x+n-I(t))\cap\Omega\right)\right)dt\right|^q dx\right\}^{1/q}\\ &\le\int_{[0,1]^d}\left\{\int_{\mathbb{T}^d}\left|\sum_{n\in\mathbb{Z}^d}\mu\left((x+n-I(t))\cap\Omega\right)\right|^q dx\right\}^{1/q}dt.\quad\square\end{aligned}$$

The following are a few applications.

Corollary 5. *Let $\gamma=4$ if $d=2$, $\gamma=3/2$ if $d=3$, $\gamma=2/(d+1)$ if $d\ge4$. Then there is a constant c depending only on the dimension d such that for every $N\ge2$ there exists a finite sequence of points $\{x_j\}_{j=1}^N$ in $[0,1]^d$ with the following property: for every convex set Ω contained in $[0,1]^d$ and for every smooth function f on $\mathbb{T}^d$,*

$$\begin{aligned}&\left|N^{-1}\sum_{j=1}^N\chi_\Omega(x_j)f(x_j)-\int_\Omega f(x)dx\right|\\ &\le cN^{-2/(d+1)}\log^\gamma(N)\sum_{\alpha\in\{0,1\}^d}\int_{[0,1]^d}\left|\left(\frac{\partial}{\partial x}\right)^{\alpha}f(x)\right|dx.\end{aligned}$$

Proof. Apply Theorem 1 to the measure $d\mu = N^{-1}\sum_{j=1}^{N}\delta_{x_j} - dx$ with $p = 1$ and $q = +\infty$. By results in [2,14], there exist sequences of points with isotropic discrepancy, that is, discrepancy of convex sets,

$$\sup_{\text{convex } A\subseteq[0,1]^d}\left\{\left|N^{-1}\sum_{j=1}^{N}\chi_A\left(x_j\right) - |A|\right|\right\} \leq cN^{-2/(d+1)}\log^{\gamma}(N). \quad \square$$

Any discrepancy is measured with respect to a given family of bodies, and of course reducing this family decreases the discrepancy. If the class of all convex bodies is replaced by the class of convex polyhedra with faces perpendicular to a given finite set of directions, then one can find sequences with a significantly smaller discrepancy.

Corollary 6. *Let $\gamma = 1$ if $d = 2$ and $\gamma = d$ if $d \geq 3$. Then for every finite set of directions Φ there exists a constant c with the following property: for every prime number $N \geq 2$ there exists a finite sequence of points $\{x_j\}_{j=1}^{N}$ in $[0, 1]^d$ such that for every convex polyhedron Ω contained in $[0, 1]^d$ and with faces perpendicular to directions in Φ, and for every smooth function f on $\mathbb{T}^d$,*

$$\begin{aligned}&\left|N^{-1}\sum_{j=1}^{N}\chi_{\Omega}\left(x_j\right)f\left(x_j\right) - \int_{\Omega}f(x)dx\right| \\ &\quad \leq cN^{-1}\log^{\gamma}(N)\sum_{\alpha\in\{0,1\}^d}\int_{[0,1]^d}\left|\left(\frac{\partial}{\partial x}\right)^{\alpha}f(x)\right|dx.\end{aligned}$$

Proof. Add the directions of the coordinate axes to the set Φ. Then for every interval I with edges parallel to the axes, all the faces of the polyhedra $I \cap \Omega$ are perpendicular to some of the directions in this new set. Then one can apply Corollary 2.11 in [4] and deduce the existence of a finite sequence $\left\{x_j\right\}_{j=1}^{N}$ with discrepancy

$$\sup_{I\subseteq[0,1]^d}\left\{\left|N^{-1}\sum_{j=1}^{N}\chi_{I\cap\Omega}\left(x_j\right) - |I\cap\Omega|\right|\right\} \leq cN^{-1}\log^{d}(N).$$

When $d = 2$, Theorem 1 in [3] gives the better estimate $cN^{-1}\log(N)$. $\square$

The following is another analog of Theorem 1, with a larger variation but a smaller discrepancy.

Theorem 7. *If $0 < a < 1$ is an irrational number and if there exist $\delta > 0$ and $\gamma \geq 2$ with the property that $|a - h/k| \geq \delta k^{-\gamma}$ for every rational h/k, then there exists a constant $c > 0$, which depends explicitly on δ, γ, d, with the following property: if $A = [-a/2, a/2]^d$ is the cube centered at the origin with side length a, if Ω is a Borel set in $\mathbb{R}^d$, if μ is a periodic Borel measure, and if f is a periodic smooth function, then*

$$\begin{aligned}\left|\int_{\Omega}f(x)\overline{d\mu(x)}\right| &\leq c\left\{\int_{\mathbb{T}^d}\left|\sum_{n\in\mathbb{Z}^d}\mu\left((x+n-A)\cap\Omega\right)\right|^2 dx\right\}^{1/2} \\ &\quad\times\left\{\sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}(1+|n_k|)^{2\gamma}\right)\left|\widehat{f}(n)\right|^2\right\}^{1/2}.\end{aligned}$$

Proof. The periodization of χ_A has Fourier expansion

$$g(x) = \sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}\frac{\sin(\pi a n_k)}{\pi n_k}\right)e^{2\pi i n\cdot x}.$$

By Lemma 2 applied to the periodization ν of the measure $\chi_{\Omega}\mu$,

$$\left|\int_{\Omega} f(x)\overline{d\mu(x)}\right| \leq \left\{\int_{\mathbb{T}^d} |g*\nu(x)|^2\,dx\right\}^{1/2} \times \left\{\int_{\mathbb{T}^d} \left|\sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}\frac{\sin(\pi a n_k)}{\pi n_k}\right)^{-1}\widehat{f}(n)e^{2\pi i n\cdot x}\right|^2 dx\right\}^{1/2}.$$

As in the proof of Theorem 1,

$$\left\{\int_{\mathbb{T}^d} |g*\nu(x)|^2\,dx\right\}^{1/2} = \left\{\int_{\mathbb{T}^d}\left|\sum_{n\in\mathbb{Z}^d}\mu\left((x+n-A)\cap\Omega\right)\right|^2 dx\right\}^{1/2}.$$

By the assumptions, $|\sin(\pi a n_k)| \geq c\,|n_k|^{1-\gamma}$ when $n_k \neq 0$. Then

$$\left|\prod_{k=1}^{d}\frac{\sin(\pi a n_k)}{\pi n_k}\right|^{-1} \leq c\prod_{k=1}^{d}(1+|n_k|)^{\gamma}.$$

Hence, by Parseval's equality,

$$\begin{aligned}&\left\{\int_{\mathbb{T}^d}\left|\sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}\frac{\sin(\pi a n_k)}{\pi n_k}\right)^{-1}\widehat{f}(n)e^{2\pi i n\cdot x}\right|^2 dx\right\}^{1/2}\\ &= \left\{\sum_{n\in\mathbb{Z}^d}\left|\left(\prod_{k=1}^{d}\frac{\sin(\pi a n_k)}{\pi n_k}\right)^{-1}\widehat{f}(n)\right|^2\right\}^{1/2}\\ &\leq c\left\{\sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}(1+|n_k|)^{2\gamma}\right)\left|\widehat{f}(n)\right|^2\right\}^{1/2}. \quad \square\end{aligned}$$

Note that the last term can be seen as the L^2 norm of a fractional derivative of order γd. If a is a quadratic irrational one can take $\gamma = 2$ and δ can be made explicit, and the variation of the function can be controlled by square norms of derivatives up to the order $2d$. This variation is larger than the one in the proof of Theorem 1, which is controlled by derivatives of order d. On the other hand, the discrepancy associated with the family of all intervals in Theorem 1 is larger than the discrepancy associated with the translates of a single cube in Theorem 7. Finally, there is an analog of the above theorem with balls instead of cubes. The zeros of Fourier transforms of characteristic functions of cubes play a crucial role in the above theorem. The Fourier transforms of balls can be expressed in terms of Bessel functions, and the following lemma is about the zeros of Bessel functions. For a reference on these special functions see [10,13].

Lemma 8. *If J_α is the Bessel function of first kind of order $\alpha \geq -1/2$, if $\beta > 5/4$, and if $0 < a < b$, then there exist $c > 0$ and $a < r < b$ with the property that for every positive integer k,*

$$\left|J_\alpha\left(r\sqrt{k}\right)\right| \geq ck^{-\beta}.$$

Proof. The zeros of $J_\alpha(t)$ are simple, with the possible exception of $t = 0$. If $\varepsilon < 1$ then $|J_\alpha(t)|^{-\varepsilon}$ is locally integrable in $t > 0$ and, by the asymptotic expansion of Bessel functions,

$$\begin{aligned}\int_a^b \left|\sqrt{r\sqrt{k}}J_\alpha\left(r\sqrt{k}\right)\right|^{-\varepsilon} dr &= k^{-1/2}\int_{a\sqrt{k}}^{b\sqrt{k}}\left|\sqrt{t}J_\alpha(t)\right|^{-\varepsilon} dt\\ &= k^{-1/2}\int_{a\sqrt{k}}^{b\sqrt{k}}\left|\sqrt{2/\pi}\cos(t-\alpha\pi/2-\pi/4)+O\left(t^{-1}\right)\right|^{-\varepsilon} dt \leq c.\end{aligned}$$

Hence, if $\varepsilon < 1$ and $\eta > 1 + \varepsilon/4$,

$$\int_a^b \left(\sum_{k=1}^{+\infty} k^{-\eta} \left| J_\alpha \left(r\sqrt{k} \right) \right|^{-\varepsilon} \right) dr \le b^{\varepsilon/2} \sum_{k=1}^{+\infty} k^{\varepsilon/4-\eta} \left(\int_a^b \left| \sqrt{r\sqrt{k}} J_\alpha \left(r\sqrt{k} \right) \right|^{-\varepsilon} dr \right) < +\infty.$$

Hence the series $\sum_{k=1}^{+\infty} k^{-\eta} \left| J_\alpha \left(r\sqrt{k} \right) \right|^{-\varepsilon}$ converges for almost every r. Then, for almost every r there exists $c > 0$ such that

$$\left| J_\alpha \left(r\sqrt{k} \right) \right| \ge ck^{-\eta/\varepsilon}. \quad \square$$

We believe that the lower bound $\beta > 5/4$ in the statement of the above lemma is not the best possible. Anyhow, the following argument shows that the lemma does not hold with $\beta < 3/4$. Assume that the interval $r\sqrt{k} \le t \le r\sqrt{k+1}$ contains a zero of $J_\alpha(t)$, that is $J_\alpha \left(r\sqrt{k+\varepsilon} \right) = 0$ with $0 \le \varepsilon \le 1$. Then for some $0 \le \eta \le \varepsilon$,

$$\begin{aligned}
\left| J_\alpha \left(r\sqrt{k} \right) \right| &= \left| J_\alpha \left(r\sqrt{k+\varepsilon} \right) - J_\alpha \left(r\sqrt{k} \right) \right| \\
&= \left| J'_\alpha \left(r\sqrt{k+\eta} \right) \left(r\sqrt{k+\varepsilon} - r\sqrt{k} \right) \right| \\
&= \left| 2^{-1} \left(J_{\alpha-1} \left(r\sqrt{k+\eta} \right) - J_{\alpha+1} \left(r\sqrt{k+\eta} \right) \right) \left(r\sqrt{k+\varepsilon} - r\sqrt{k} \right) \right| \\
&\le 2^{-1} \left(\sup_{0<\eta<1} \left| J_{\alpha-1} \left(r\sqrt{k+\eta} \right) \right| + \sup_{0<\eta<1} \left| J_{\alpha+1} \left(r\sqrt{k+\eta} \right) \right| \right) \\
&\quad \times \left(r\sqrt{k+1} - r\sqrt{k} \right) \\
&\le c\sqrt{r} k^{-3/4}.
\end{aligned}$$

Theorem 9. *For every $0 < a < b$ and $\gamma > d/2 + 5/4$, there exist a constant $c > 0$ and a radius $a < r < b$ with the following properties: if $B = \{|x| \le r\}$ is the ball centered at the origin with radius r, if Ω is a Borel set in $\mathbb{R}^d$, if μ is a periodic Borel measure, and if f is a periodic smooth function, then*

$$\begin{aligned}
\left| \int_\Omega f(x) \overline{d\mu(x)} \right| &\le c \left\{ \int_{\mathbb{T}^d} \left| \sum_{n \in \mathbb{Z}^d} \mu\left((x+n-B) \cap \Omega \right) \right|^2 dx \right\}^{1/2} \\
&\quad \times \left\{ \sum_{n \in \mathbb{Z}^d} \left(1 + |n|^2 \right)^\gamma \left| \widehat{f}(n) \right|^2 \right\}^{1/2}.
\end{aligned}$$

Proof. The Fourier transform of the characteristic function of a ball is a Bessel function, and the periodization of χ_B has Fourier expansion

$$g(x) = \sum_{n \in \mathbb{Z}^d} r^{d/2} |n|^{-d/2} J_{d/2}(2\pi r |n|) e^{2\pi i n \cdot x}.$$

See Theorem 4.15 in Chapter IV of [13]. By Lemma 2 applied to the periodization ν of the measure $\chi_\Omega \mu$,

$$\begin{aligned}
\left| \int_\Omega f(x) \overline{d\mu(x)} \right| &\le \left\{ \int_{\mathbb{T}^d} |g * \nu(x)|^2 dx \right\}^{1/2} \\
&\quad \times \left\{ \int_{\mathbb{T}^d} \left| \sum_{n \in \mathbb{Z}^d} \left(r^{d/2} |n|^{-d/2} J_{d/2}(2\pi r |n|) \right)^{-1} \widehat{f}(n) e^{2\pi i n \cdot x} \right|^2 dx \right\}^{1/2}.
\end{aligned}$$

As in the proof of Theorem 1,

$$\left\{\int_{\mathbb{T}^d} |g * \nu(x)|^2 \, dx\right\}^{1/2} = \left\{\int_{\mathbb{T}^d} \left|\sum_{n\in\mathbb{Z}^d} \mu\left((x+n-B)\cap\Omega\right)\right|^2 dx\right\}^{1/2}.$$

Moreover, by Parseval's equality and Lemma 8, one can choose r so that

$$\begin{aligned}
&\left\{\int_{\mathbb{T}^d} \left|\sum_{n\in\mathbb{Z}^d} \left(r^{d/2}\,|n|^{-d/2} J_{d/2}\left(2\pi r\,|n|\right)\right)^{-1} \widehat{f}(n) e^{2\pi i n\cdot x}\right|^2 dx\right\}^{1/2} \\
&\quad = \left\{\sum_{n\in\mathbb{Z}^d} \left|\left(r^{d/2}\,|n|^{-d/2} J_{d/2}\left(2\pi r\,|n|\right)\right)^{-1} \widehat{f}(n)\right|^2\right\}^{1/2} \\
&\quad \le c\left\{\sum_{n\in\mathbb{Z}^d} \left(1+|n|^2\right)^{\gamma} \left|\widehat{f}(n)\right|^2\right\}^{1/2}. \quad \square
\end{aligned}$$

Since less than $d/2$ square integrable derivatives are not enough to guarantee the boundedness of a function, in the above theorem the assumption $\gamma > d/2+5/4$ is not too far from being best possible.

3. Koksma–Hlawka inequalities on manifolds

The results in the previous section are of local nature and with a change of variables they can be easily transferred from cubes to compact manifolds. Let $\mathcal{M}$ be a smooth compact d-dimensional manifold with a normalized measure dx. Choose a family of local charts $\{\varphi_k\}_{k=1}^K$, $\varphi_k : [0,1]^d \to \mathcal{M}$, and a smooth partition of unity $\{\psi_k\}_{k=1}^K$ subordinate to these charts. The Sobolev spaces $W^{n,p}(\mathcal{M})$ can be defined by the norms

$$\|f\|_{W^{n,p}(\mathcal{M})} = \sum_{1\le k\le K}\sum_{|\alpha|\le n}\left\{\int_{[0,1]^d}\left|\frac{\partial^\alpha}{\partial x^\alpha}\left(\psi_k\left(\varphi_k(x)\right) f\left(\varphi_k(x)\right)\right)\right|^p dx\right\}^{1/p}.$$

One can define an interval in $\mathcal{M}$ as the image under a local chart of an interval in $[0,1]^d$, say $U = \varphi_k(I)$. The discrepancy of a finite Borel measure μ on $\mathcal{M}$ with respect to the collection A of all intervals in $\mathcal{M}$ is

$$\mathcal{D}(\mu) = \sup_{U\in A}\left|\int_U d\mu(y)\right|.$$

Theorem 10. *There exists a constant $c > 0$, which depends on the local charts but not on the function f or the measure μ, such that*

$$\left|\int_{\mathcal{M}} f(y)\overline{d\mu(y)}\right| \le c\mathcal{D}(\mu)\,\|f\|_{W^{d,1}(\mathcal{M})}.$$

Proof. It suffices to prove the theorem for a function with support in the image of a single local chart $\varphi : [0,1]^d \to \mathcal{M}$. If the measure ν is the pull back on $[0,1]^d$ of the measure μ on $\mathcal{M}$ then, by Theorem 1,

$$\begin{aligned}
\left|\int_{\mathcal{M}} f(y)\overline{d\mu(y)}\right| &= \left|\int_{[0,1]^d} f\left(\varphi(x)\right)\overline{d\nu(x)}\right| \\
&\le 2^d\left\{\sup_{I\subseteq[0,1]^d}\left|\int_{[0,1]^d}\chi_I(x)d\nu(x)\right|\right\} \\
&\quad \times\left\{\sum_{\alpha\in\{0,1\}^d} 2^{d-|\alpha|}\int_{[0,1]^d}\left|\left(\frac{\partial}{\partial x}\right)^\alpha f\left(\varphi(x)\right)\right| dx\right\}.
\end{aligned}$$

The first factor is dominated by the discrepancy,

$$\sup_{I\subseteq[0,1]^d}\left\{\left|\int_{[0,1]^d}\chi_I(x)d\nu(x)\right|\right\}\leq\sup_{U\in A}\left\{\left|\int_{\mathcal{M}}\chi_U(y)d\mu(y)\right|\right\}.$$

The second factor is dominated by the Sobolev norm,

$$\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\int_{[0,1]^d}\left|\left(\frac{\partial}{\partial x}\right)^{\alpha}f\left(\varphi(x)\right)\right|dx\leq c\,\|f\|_{W^{d,1}(\mathcal{M})}.\quad\square$$

As an example, consider the 2-dimensional sphere. If the local charts are gnomonic projections, that is central projections from the tangent planes to the sphere, then the straight lines on the tangent planes are mapped into the great circles of the sphere. In particular, since a quadrilateral is the union of two triangles, the discrepancy with respect to quadrilaterals can be controlled by the discrepancy with respect to geodesic triangles. Finally, as in Theorem 9, one can consider a Koksma–Hlawka inequality on the sphere, with spherical cap discrepancy. The zonal polynomials $Z_n\left(x\cdot y\right)$ on the sphere $\mathcal{S}=\left\{x\in\mathbb{R}^3:|x|=1\right\}$ are the reproducing kernels of the spaces of harmonic polynomials of degree n. If $Q_n(x)$ is a harmonic polynomial of degree n, then

$$Q_n(x)=\int_{\mathcal{S}}Z_n\left(x\cdot y\right)Q_n(y)dy.$$

Every distribution f on the sphere has a spherical harmonic expansion

$$f(x)=\sum_{n=0}^{+\infty}\int_{\mathcal{S}}Z_n\left(x\cdot y\right)f(y)dy=\sum_{n=0}^{+\infty}\widehat{f}\left(n,x\right).$$

The series converges in the topology of distributions. If f is square integrable, the series converges in the square norm, and if it is smooth, it also converges absolutely and uniformly. As a reference on the harmonic analysis on the sphere and for the properties of the zonal polynomials that will be needed in what follows, see [10,13]. The following is a spherical analog of Lemma 2.

Lemma 11. *Let f be a smooth function and μ a finite measure on the sphere. Also let $\varphi(n)$ be a non vanishing complex sequence on $\mathbb{N}$, and assume that both $\varphi(n)$ and $1/\varphi(n)$ have tempered growth. Define*

$$\mathfrak{D}f(x)=\sum_{n=0}^{+\infty}\varphi(n)\widehat{f}\left(n,x\right),$$
$$g\left(x\cdot y\right)=\sum_{n=0}^{+\infty}\overline{\varphi\left(n\right)^{-1}}Z_n\left(x\cdot y\right).$$

Then

$$\left|\int_{\mathcal{S}}f(x)\overline{d\mu(x)}\right|\leq\left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}g\left(x\cdot y\right)d\mu(y)\right|^2dx\right\}^{1/2}\left\{\int_{\mathcal{S}}\left|\mathfrak{D}f\left(x\right)\right|^2dx\right\}^{1/2}.$$

Proof. By the spherical harmonic expansions of f and μ,

$$\begin{aligned}\left|\int_{\mathcal{S}}f(x)\overline{d\mu(x)}\right|&=\left|\sum_{n=0}^{+\infty}\int_{\mathcal{S}}\widehat{f}\left(n,x\right)\overline{\widehat{\mu}\left(n,x\right)}dx\right|\\&\leq\left\{\int_{\mathcal{S}}\left|\sum_{n=0}^{+\infty}\varphi\left(n\right)\widehat{f}\left(n,x\right)\right|^2dx\right\}^{1/2}\\&\quad\times\left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}\left(\sum_{n=0}^{+\infty}\overline{\varphi(n)^{-1}}Z_n\left(x\cdot y\right)\right)d\mu(y)\right|^2dx\right\}^{1/2}.\quad\square\end{aligned}$$

Here we consider two specific examples of sequences φ and functions g. The following is an analog of Lemma 8, with Legendre polynomials in place of Bessel functions.

Lemma 12. (1) *Let*

$$\chi_{\{x\cdot y\geq\cos(\vartheta)\}}\left(x\cdot y\right)=\sum_{n=0}^{+\infty}\overline{\varphi(n)^{-1}}Z_n\left(x\cdot y\right)$$

be the spherical harmonic expansion of the characteristic function of the spherical cap $\{x\cdot y\geq\cos(\vartheta)\}$ *on the* 2*-dimensional sphere. Then for every* $\gamma>5/2$ *and for almost every* $0<\vartheta<\pi$ *there exist positive constants* c_1 *and* c_2 *such that for every positive integer* n*,*

$$c_1n^{3/2}\leq|\varphi(n)|\leq c_2n^{\gamma}.$$

(2) *Let*

$$\chi_{\{x\cdot y\geq\cos(\vartheta)\}}\left(x\cdot y\right)+i\chi_{\{x\cdot y\geq\cos(2\vartheta)\}}\left(x\cdot y\right)=\sum_{n=0}^{+\infty}\overline{\varphi(n)^{-1}}Z_n\left(x\cdot y\right).$$

Then for almost every $0<\vartheta<\pi/2$ *there exist positive constants* c_1 *and* c_2 *such that for every positive integer* n*,*

$$c_1n^{3/2}\leq|\varphi(n)|\leq c_2n^{3/2}.$$

Proof. The zonal polynomials on the sphere are multiples of Legendre polynomials,

$$Z_n\left(x\cdot y\right)=\left(2n+1\right)P_n\left(x\cdot y\right),$$

$$P_n(z)=\frac{d^n}{dz^n}\frac{\left(z^2-1\right)^n}{2^nn!}.$$

The characteristic function of the spherical cap $\{x\cdot y\geq\cos(\vartheta)\}$ has the expansion,

$$\begin{aligned}\chi_{\{x\cdot y\geq\cos(\vartheta)\}}\left(x\cdot y\right)&=\sum_{n=0}^{+\infty}\left(\left(n+1/2\right)\int_{\cos(\vartheta)}^{1}P_n(z)dz\right)P_n\left(x\cdot y\right)\\&=\frac{1-\cos(\vartheta)}{2}+\sum_{n=1}^{+\infty}\frac{P_{n-1}\left(\cos(\vartheta)\right)-P_{n+1}\left(\cos(\vartheta)\right)}{2}P_n\left(x\cdot y\right)\\&=\frac{1-\cos(\vartheta)}{2}Z_0\left(x\cdot y\right)+\sum_{n=1}^{+\infty}\frac{P_{n-1}\left(\cos(\vartheta)\right)-P_{n+1}\left(\cos(\vartheta)\right)}{2\left(2n+1\right)}Z_n\left(x\cdot y\right).\end{aligned}$$

See [10, 4.8]. This follows from the identities

$$Z_n(z)=\left(2n+1\right)P_n(z)=P'_{n+1}(z)-P'_{n-1}(z).$$

Therefore $\varphi(0)^{-1}=\left(1-\cos(\vartheta)\right)/2$ and, if $n=1,2,3,\ldots$

$$\varphi(n)^{-1}=\frac{P_{n-1}\left(\cos(\vartheta)\right)-P_{n+1}\left(\cos(\vartheta)\right)}{2\left(2n+1\right)}.$$

The Legendre polynomials in $0<a<\vartheta<b<\pi$ have the asymptotic expansion

$$P_n\left(\cos(\vartheta)\right)=\sqrt{\frac{2}{\pi n\sin(\vartheta)}}\cos\left(\left(n+1/2\right)\vartheta+\pi/4\right)+O\left(n^{-3/2}\right).$$

See [10, 4.6]. Hence

$$
\begin{aligned}
P_{n-1}(\cos(\vartheta)) - P_{n+1}(\cos(\vartheta)) &= \sqrt{\frac{2}{\pi\,(n-1)\sin(\vartheta)}}\cos((n-1/2)\,\vartheta+\pi/4) \\
&\quad - \sqrt{\frac{2}{\pi\,(n+1)\sin(\vartheta)}}\cos((n+3/2)\,\vartheta+\pi/4) + O\left(n^{-3/2}\right) \\
&= \sqrt{\frac{2}{\pi n\sin(\vartheta)}}\left(\cos((n-1/2)\,\vartheta+\pi/4) - \cos((n+3/2)\,\vartheta+\pi/4)\right) + O\left(n^{-3/2}\right) \\
&= \sqrt{\frac{2}{\pi n\sin(\vartheta)}}2\sin(\vartheta)\sin((n+1/2)\,\vartheta+\pi/4) + O\left(n^{-3/2}\right).
\end{aligned}
$$

Actually, we need a slightly more precise estimate. Observe that the above polynomial vanishes only when $(n+1/2)\,\vartheta+\pi/4$ is close to a multiple of π, but at these points the derivative is large,

$$
\begin{aligned}
&\frac{d}{d\vartheta}\left(P_{n-1}(\cos(\vartheta)) - P_{n+1}(\cos(\vartheta))\right) = (2n+1)\sin(\vartheta)\,P_n(\cos(\vartheta)) \\
&\quad = (2n+1)\sqrt{\frac{2\sin(\vartheta)}{\pi n}}\cos((n+1/2)\,\vartheta+\pi/4) + O\left(n^{-1/2}\right).
\end{aligned}
$$

In particular, if n is large, say $n \geq N$, and $0 < a < \vartheta < b < \pi$ then the zeros are simple. This implies that

$$
\varphi(n)^{-1} = \frac{\sqrt{2\sin(\vartheta)}\left(\sin((n+1/2)\,\vartheta+\pi/4) + O(1/n)\right)}{\sqrt{\pi n}\,(2n+1)}.
$$

It follows from these estimates that $\left|\varphi(n)^{-1}\right| \leq cn^{-3/2}$ for every ϑ, that is $|\varphi(n)| \geq cn^{3/2}$. Finally, in order to prove a reverse inequality one can argue as in the proof of Lemma 8. If $\varepsilon < 1$ and $\eta > 1+3\varepsilon/2$, then

$$
\int_a^b \left(\sum_{n=N}^{+\infty} n^{-\eta}\,|\varphi(n)|^{\varepsilon}\right) d\vartheta < +\infty.
$$

Hence, the series $\sum_{n=1}^{+\infty} n^{-\eta}\,|\varphi(n)|^{\varepsilon}$ converges for almost every ϑ, then for almost every ϑ there exists $c > 0$ such that

$$
|\varphi(n)| \leq cn^{\eta/\varepsilon}.
$$

This proves (1). The proof of (2) is a bit different. Let

$$
\chi_{\{x\cdot y\geq\cos(\vartheta)\}}(x\cdot y) + i\chi_{\{x\cdot y\geq\cos(2\vartheta)\}}(x\cdot y) = \sum_{n=0}^{+\infty}\overline{\varphi(n)^{-1}}Z_n(x\cdot y).
$$

Then, if $n = 1, 2, 3, \ldots,$

$$
\begin{aligned}
|\varphi(n)| &= \left|\frac{P_{n-1}(\cos(\vartheta)) - P_{n+1}(\cos(\vartheta))}{2\,(2n+1)} + i\frac{P_{n-1}(\cos(2\vartheta)) - P_{n+1}(\cos(2\vartheta))}{2\,(2n+1)}\right|^{-1} \\
&= \left(\left|\frac{P_{n-1}(\cos(\vartheta)) - P_{n+1}(\cos(\vartheta))}{2\,(2n+1)}\right|^2 + \left|\frac{P_{n-1}(\cos(2\vartheta)) - P_{n+1}(\cos(2\vartheta))}{2\,(2n+1)}\right|^2\right)^{-1/2} \\
&= \sqrt{\pi n/2}\,(2n+1)\Big(|\sin(\vartheta)|\sin^2((n+1/2)\,\vartheta+\pi/4) \\
&\quad + |\sin(2\vartheta)|\sin^2((2n+1)\,\vartheta+\pi/4) + O(1/n)\Big)^{-1/2}.
\end{aligned}
$$

If $0 < a < \vartheta < b < \pi/2$ and if n is large, then

$$\begin{aligned}
&|\sin(\vartheta)|\sin^2((n+1/2)\vartheta+\pi/4)+|\sin(2\vartheta)|\sin^2((2n+1)\vartheta+\pi/4)+O(1/n)\\
&\quad\geq c\left(\sin^2((n+1/2)\vartheta+\pi/4)+\sin^2((2n+1)\vartheta+\pi/4)\right)+O(1/n)\\
&\quad\geq c\min_{0\leq\omega\leq\pi}\left\{\sin^2(\omega)+\sin^2(2\omega-\pi/4)\right\}+O(1/n)\geq c>0.
\end{aligned}$$

In particular, there exists N such that for every $n \geq N$ and every $0 < a < \vartheta < b < \pi/2$, one has $|\varphi(n)| \leq cn^{3/2}$. Moreover, the equations $\varphi(n) = 0$ for some $n < N$ have a finite number of solutions in $0 < a < \vartheta < b < \pi/2$. Hence, if ϑ is not one of these solutions, then it satisfies (2). □

Theorem 13. (1) *For every $\gamma > 5/2$ and almost every $0 < \vartheta < \pi$ there exists a constant $c > 0$ with the following property: if $B(x, \vartheta) = \{x \cdot y \geq \cos(\vartheta)\}$ are the spherical caps with center x and radius ϑ, if Ω is a Borel set, if μ is a Borel measure, and if f is a smooth function in $\mathcal{S}$, then*

$$\left|\int_\Omega f(x)\overline{d\mu(x)}\right| \leq c\left\{\int_{\mathcal{S}}|\mu(B(x,\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}\left\{\sum_{n=0}^{+\infty}\left(1+n^2\right)^\gamma\int_{\mathcal{S}}\left|\widehat{f}(n,x)\right|^2 dx\right\}^{1/2}.$$

(2) *For almost every radius $0 < \vartheta < \pi/2$ there exists a constant $c > 0$ with the property that*

$$\begin{aligned}
\left|\int_\Omega f(x)\overline{d\mu(x)}\right| \leq\ & c\left\{\sum_{n=0}^{+\infty}\left(1+n^2\right)^{3/2}\int_{\mathcal{S}}\left|\widehat{f}(n,x)\right|^2 dx\right\}^{1/2}\\
&\times\left(\left\{\int_{\mathcal{S}}|\mu(B(x,\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}\right.\\
&\left.+\left\{\int_{\mathcal{S}}|\mu(B(x,2\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}\right).
\end{aligned}$$

Proof. If $g(x\cdot y) = \chi_{\{x\cdot y\geq\cos(\vartheta)\}}(x\cdot y)$ and if ν is the restriction of the measure μ to the set Ω,

$$\left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}g(x\cdot y)\,d\nu(y)\right|^2 dx\right\}^{1/2} = \left\{\int_{\mathcal{S}}|\mu(B(x,\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}.$$

Then (1) follows from Lemmas 11 and 12(1). If $g(x\cdot y) = \chi_{\{x\cdot y\geq\cos(\vartheta)\}}(x\cdot y) + i\chi_{\{x\cdot y\geq\cos(2\vartheta)\}}(x\cdot y)$ and if ν is the restriction of the measure μ to the set Ω,

$$\begin{aligned}
\left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}g(x\cdot y)\,d\nu(y)\right|^2 dx\right\}^{1/2} &\leq \left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}\chi_{\{x\cdot y\geq\cos(\vartheta)\}}(x\cdot y)\,d\nu(y)\right|^2 dx\right\}^{1/2}\\
&\quad+\left\{\int_{\mathcal{S}}\left|\int_{\mathcal{S}}\chi_{\{x\cdot y\geq\cos(2\vartheta)\}}(x\cdot y)\,d\nu(y)\right|^2 dx\right\}^{1/2}\\
&=\left\{\int_{\mathcal{S}}|\mu(B(x,\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}\\
&\quad+\left\{\int_{\mathcal{S}}|\mu(B(x,2\vartheta)\cap\Omega)|^2\,dx\right\}^{1/2}.
\end{aligned}$$

Then, as before, (2) follows from Lemmas 11 and 12(2). □

Observe that the indices $\gamma > 9/4$ in Theorem 9 with $d = 2$ and $\gamma > 5/2$ in Theorem 13(1) are different. Anyhow, it is likely that both indices are not best possible. Finally, an analog of Theorem 13(1) holds on spheres of dimension $d > 2$ with $\gamma > (d+3)/2$.

4. An application

In order to test the quality of the above results, we reconsider an example in [6]. Let

$$f\left(x_1, x_2, \ldots, x_d\right) = \frac{1}{x_1 x_2 \cdots x_d \left(1 - x_1 - x_2 - \cdots - x_d\right)}.$$

Also, for $\varepsilon > 0$ small, let Σ be the simplex

$$\Sigma = \left\{ \left(x_1, \ldots, x_d\right) \in \mathbb{R}^d : x_1 \geq \cdots \geq x_d \geq \varepsilon,\ 1 - x_1 - \cdots - x_d \geq \varepsilon \right\}.$$

One can show that

$$\sum_{|\alpha| \leq d} \int_{\Sigma} \left| \left(\frac{\partial}{\partial x} \right)^{\alpha} f(x) \right| dx \leq c\varepsilon^{-d}.$$

By Corollary 5 there exists a finite sequence $\left\{x_j\right\}_{j=1}^{N}$ in $[0, 1]^d$ such that for all convex sets Ω contained in Σ,

$$\left| N^{-1} \sum_{j=1}^{N} \left(f \chi_{\Omega}\right)\left(x_j\right) - \int_{\Omega} f(x) dx \right| \leq c\varepsilon^{-d} N^{-2/(d+1)} \log^{\gamma}(N).$$

This agrees with the result in [6]. However, in the case $\Omega = \Sigma$, Corollary 6 gives the better estimate

$$\left| N^{-1} \sum_{j=1}^{N} \left(f \chi_{\Sigma}\right)\left(x_j\right) - \int_{\Sigma} f(x) dx \right| \leq c\varepsilon^{-d} N^{-1} \log^{d}(N).$$

References

[1] C. Amstler, P. Zinterhof, Uniform distribution, discrepancy, and reproducing kernel Hilbert spaces, Journal of Complexity 17 (2001) 497–515.
[2] J. Beck, On the discrepancy of convex plane sets, Monatshefte für Mathematik 105 (1988) 91–106.
[3] W.W.L. Chen, G. Travaglini, Discrepancy with respect to convex polygons, Journal of Complexity 23 (2007) 662–672.
[4] L. Colzani, G. Gigante, G. Travaglini, Trigonometric approximation and a general form of the Erdős–Turan inequality, Transactions of the American Mathematical Society 363 (2011) 1101–1123.
[5] G. Harman, Metric Number Theory, Oxford University Press, New York, 1998.
[6] G. Harman, Variations on the Koksma–Hlawka inequality, Uniform Distribution Theory 5 (2010) 65–78.
[7] F.J. Hickernell, Koksma–Hlawka inequality, in: S. Kotz, C.B. Read, D.L. Banks (Eds.), Encyclopedia of Statistical Sciences, Wiley-Interscience, John Wiley & Sons, New York, London, Sydney, 2006.
[8] E. Hlawka, The Theory of Uniform Distribution, A B Academic Publishers, Berkhamsted, 1984.
[9] L. Kuipers, H. Niederreiter, Uniform Distribution of Sequences, Dover Publications, New York, 2006.
[10] N.N. Lebedev, Special Functions & their Applications, Dover Publications, New York, 1972.
[11] J. Matoušek, Geometric Discrepancy, An Illustrated Guide, Springer-Verlag, Berlin, 2010.
[12] H. Niederreiter, Random Number Generation and Quasi-Monte Carlo Methods, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, 1992.
[13] E.M. Stein, G. Weiss, Introduction to Fourier Analysis on Euclidean spaces, Princeton University Press, Princeton, 1971.
[14] W. Stute, Convergence rates for the isotrope discrepancy, Annals of Probability 5 (1977) 707–723.
[15] G. Travaglini, Appunti su Teoria dei Numeri, Analisi di Fourier e Distribuzione di Punti, Unione Matematica Italiana, Pitagora Editrice, Bologna, 2010.
[16] S.K. Zaremba, Some applications of multidimensional integration by parts, Annales Polonici Mathematici 21 (1968) 85–96.