Discrepancies of Point Sequences on the Sphere and Numerical Integration

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Abstract

Several concepts of discrepancy for point sequences on the d-dimensional unit sphere S^d are studied. The different discrepancies are compared to each other and applied to error estimates in numerical integration.

0 Introduction

Numerical integration of continuous functions on the d-dimensional unit sphere S^d is an important application of Quasi-Monte Carlo methods. In principal, one has to generate a sequence of points $\mathbf{x}_n$, $n = 1, \ldots, N$ on the sphere in order to approximate the integral

$$I(f) = \int\limits_{S^d} f(\mathbf{x})\, d\sigma(\mathbf{x})$$

by functionals

$$I_N(f) = \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n),$$

where σ denotes the normalized surface measure on S^d and f is a continuous real valued function. As a general reference on Quasi-Monte Carlo methods we mention Niederreiter [22]. The problem of distributing points on the sphere is also related to constructive multivariate approximation, see Reimer [24]. For the recent literature on spherical problems concerned with approximation and numerical integration we refer to the forthcoming book [7].

For applications in numerical integration it is necessary to have suitably smoothly distributed points on the sphere. There are several quantities measuring the distribution of point sets $\mathbf{x}_n$, $n = 1, \ldots, N$. The geometrically most natural concept is the spherical cap discrepancy

$$D_N^C(\mathbf{x}_n) := \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(\mathbf{x}_n) - \sigma(C) \right|, \tag{0.1}$$

where a spherical cap with center $\mathbf{y}$ and radius ϕ is defined as $C := \{\mathbf{x} : \langle \mathbf{x}, \mathbf{y} \rangle > \cos\phi\}$ which is the intersection of the sphere and a half space; χ_C denotes the characteristic function of C. (Here and in the following we consider S^d to be embedded in $\mathbb{R}^{d+1}$ and $\langle \cdot, \cdot \rangle$ denotes the standard inner product on $\mathbb{R}^{d+1}$.) Roughly speaking, this discrepancy measures the maximal deviation between the empirical distribution of the points and uniform distribution.

The error $E_N(f) = |I_N(f) - I(f)|$ in numerical integration of continuous functions on S^d satisfying a Lipschitz condition $|f(\mathbf{x}) - f(\mathbf{y})| \le C_f \arccos(\langle \mathbf{x}, \mathbf{y} \rangle)$ can be estimated by

$$E_N(f) \le C_f \left(\frac{6d}{M} + \pi \sum_{m=1}^{2M} \sum_{\ell=1}^{Z(d,m)} \left| \frac{1}{N} \sum_{n=1}^{N} S_{m,\ell}(\mathbf{x}_n) \right| \right),$$

where M is an arbitrary positive integer and $S_{m,\ell}$, $\ell = 1, \ldots, Z(d,m)$ denotes an orthonormal basis of the spherical harmonics of order m (cf. [20]). The proof is given in [10] and makes use of an approximation kernel due to Newman and Shapiro [21].

Extending the well known Erdös-Turán inequality (cf. [17], [14]), Grabner [9] established the following bound for the cap discrepancy: For any positive integer M and constants $c_i(d)$ only depending on the dimension d the inequality

$$D_N^C(\mathbf{x}_n) \le \frac{c_1(d)}{M+1} + \sum_{m=1}^{M} \left(\frac{c_2(d)}{m} + \frac{c_3(d)}{M+1} \right) \sum_{j=1}^{Z(d,m)} \left| \frac{1}{N} \sum_{n=1}^{N} S_{m,j}(\mathbf{x}_n) \right| \tag{0.2}$$

holds. The proof of this result mainly depends on Vaaler's approximation kernel [28], which is very suitable to approximate step functions by trigonometric polynomials.

The above upper bound for the cap discrepancy in terms of the spherical harmonics suggests that a notion of discrepancy based on spherical harmonics might be fruitful. In analogy to the so called polynomial discrepancy for sequences in $[0,1)^d$ (cf. [12], [27]) we introduce a spherical polynomial discrepancy defined by

$$D_N^S(\mathbf{x}_n) := \sup_{m \ge 1} \frac{1}{m^d} \max_{1 \le j \le Z(d,m)} \left| \frac{1}{N} \sum_{n=1}^{N} S_{m,j}(\mathbf{x}_n) \right|. \tag{0.3}$$

It is a natural question to ask whether uniform distribution of infinite point sequences can be defined via cap discrepancy as well as via the polynomial discrepancy. Let us recall the definition of uniform distribution of sequence $(\mathbf{x}_n)_{n=1}^{\infty}$: $(\mathbf{x}_n)$ is said to be uniformly distributed if

$$\lim_{N\to\infty} I_N(f) = I(f)$$

for all continuous functions f. By well known arguments (cf. [17]) this is equivalent to

$$\lim_{N\to\infty} D_N^C(\mathbf{x}_n) = 0 \quad \text{or} \quad \lim_{N\to\infty} D_N^S(\mathbf{x}_n) = 0.$$

A quantitative relation between these two concepts of discrepancy is due to Klinger and Tichy [15]

$$c_4(d) D_N^S(\mathbf{x}_n) \le D_N^C(\mathbf{x}_n) \le c_5(d) \left(D_N^S(\mathbf{x}_n) \right)^{\frac{1}{2d}} \tag{0.4}$$

with constants only depending on the dimension.

An upper bound for the cap discrepancy in terms of Legendre polynomials P_m^d was proved by Grabner and Tichy [10]:

Theorem 0.1.

$$D_N^C(\mathbf{x}_n) \le \frac{c_6(d)}{M+1} + c_7(d) \sum_{m=1}^{M} m^{\frac{d-3}{2}} \frac{1}{N} \sqrt{\sum_{i=1}^{N} \sum_{\ell=1}^{N} P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell \rangle)}.$$

Remark 1 *In the following we make frequently use of the addition theorem for spherical harmonics*

$$\sum_{j=1}^{Z(d,n)} S_{n,j}(\mathbf{x}) S_{n,j}(\mathbf{y}) = Z(d,n) P_n^d(\langle \mathbf{x}, \mathbf{y} \rangle),$$

where the Legendre polynomials are normalized such that $|P_n^d(x)| \le P_n^d(1) = 1$*. Furthermore, they are given by the generating function (cf. [19])*

$$\sum_{n=0}^{\infty} (n+1)(n+2)\cdots(n+d-2) P_n^d(t) z^n = \frac{1}{(1-2tz+z^2)^{\frac{d-1}{2}}}. \tag{0.5}$$

The numerical value of the dimension $Z(d,n)$ *is known to be* $\frac{2n+d-1}{n+d-1}\binom{n+d-1}{d-1}$.

This suggests to define a discrepancy based on Legendre polynomials:

$$D_N^P(\mathbf{x}_n) := \sup_{m\geq 1} \frac{1}{m^d} \frac{1}{N} \sqrt{\sum_{i=1}^N \sum_{\ell=1}^N P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell \rangle)}. \tag{0.6}$$

Again this discrepancy is compatible with the above mentioned concepts:

$$c_8(d) D_N^P(\mathbf{x}_n) \leq D_N^C(\mathbf{x}_n) \leq c_9(d) \left(D_N^P\right)^{\frac{2}{3d+1}},$$

where the constants depend only on the dimension (cf. [15]).

For the case $d = 2$ Freeden [8] developed a discrepancy based on the Green function $G(x, y)$ of the Beltrami operator. The Fourier series of this function is given by

$$G(\mathbf{x}, \mathbf{y}) = \sum_{n=1}^{\infty} \frac{\varphi_n(\mathbf{x})\varphi_n(\mathbf{y})}{\lambda_n},$$

where $\varphi_n(\mathbf{x})$ and λ_n are the eigenfunctions and eigenvalues of the operator. In order to make the series convergent, iterations of this kernel are considered:

$$G^{(r)}(\mathbf{x}, \mathbf{y}) = \sum_{n=1}^{\infty} \frac{\varphi_n(\mathbf{x})\varphi_n(\mathbf{y})}{\lambda_n^r}.$$

This sum is uniformly convergent for $r \geq [\frac{d+3}{2}]$. The Green discrepancy (of order r) is defined by

$$D_N^{(G,r)}(\mathbf{x}_n) := \sup_{\mathbf{y}\in S^d} \left| \frac{4\pi}{N} \sum_{n=1}^N G^{(r)}(\mathbf{x}_n, \mathbf{y}) \right| \tag{0.7}$$

and might be a suitable measure for the quality of the distribution. In fact, Hlawka [13] considered an extension of this kind of discrepancy to Riemannian manifolds and proved that the cap discrepancy is compatible with the Green function discrepancy. Hlawka [13] established the following bounds

$$c_{10}(d) \left(D_N^{(G,r)}\right)^{\frac{d+1}{2r-d-1}} \leq D_N^C \leq c_{11}(d) \left(D_N^{(G,r)}\right)^{\frac{1}{4r+2d+3}} \left|\log D_N^{(G,r)}\right|. \tag{0.8}$$

Note, that we suppose $r \geq [\frac{d+3}{2}]$. For $r > d+1$ the left hand of (0.8) can be improved to $c_{12}(d) D_N^{(G,r)}$ and for $r = d+1$ to $c_{13}(d) D_N^{(G,r)} |\log D_N^{(G,r)}|^{-1}$. The Green function discrepancy is extremely useful for estimating the approximation error $E_N(f)$ via a Koksma-Hlawka type inequality

$$E_N(f) \leq V^{(r)}(f) \cdot D_N^{(G,r)}, \tag{0.9}$$

where $V^{(r)}(f) = \int_{S^d} |\Delta^{(r)} f(\mathbf{x})| \, d\sigma(\mathbf{x})$ with $\Delta^{(r)}$ the r-times iterated Laplace-Beltrami operator, cf. [13].

A different approach was made by Cui and Freeden [5], who used elements of the theory of weighted Sobolev spaces to obtain an estimate for the approximation error in terms of the following modified polynomial discrepancy

$$\begin{aligned} D_N^{P^*}(\mathbf{x}_n) \quad &:= \quad \frac{1}{N} \left[\sum_{i=1}^{N} \sum_{\ell=1}^{N} \sum_{m=1}^{\infty} \frac{1}{m(m+1)} \, P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell \rangle) \right]^{\frac{1}{2}} \\ &= \quad \frac{1}{N} \left[\sum_{i=1}^{N} \sum_{\ell=1}^{N} \left(1 - 2 \ln \left(1 + \sqrt{\frac{1 - \langle \mathbf{x}_i, \mathbf{x}_\ell \rangle}{2}} \right) \right) \right]^{\frac{1}{2}} \end{aligned}$$

for the case $d = 2$. The concept, however, is not restricted to the case $d = 2$ and in Section 1 we will give a generalization to aribitrary dimensions. We will prove that

$$D_N^P(\mathbf{x}_n) \leq D_N^{P^*}(\mathbf{x}_n) \leq c_{14}(d) \left(D_N^P \right)^{\frac{1}{2(d+1)}} . \tag{0.10}$$

The appearance of Legendre polynomials and spherical harmonics in the expressions for discrepancies is not artificial but makes sense for another reason, namely the construction of optimally chosen integration points, so called spherical designs.

A point set $\mathbf{x}_1, \ldots, \mathbf{x}_N \in S^d$ is called a spherical t-design if

$$\frac{1}{N} \sum_{n=1}^{N} p(\mathbf{x}_n) = \int_{S^d} p(\mathbf{x}) \, d\sigma(\mathbf{x})$$

for all polynomials (in $d+1$ variables restricted to S^d) of degree not greater than t. Now, we would expect point sets which are spherical t-designs for large t to have small discrepancy. This is in fact the case; we may easily deduce from the definitions and a standard upper bound for the Legendre polynomials (cf. [19]) that for any spherical t-design $\mathbf{x}_1, \ldots, \mathbf{x}_N$ we have

$$D_N^P(\mathbf{x}_n) \ll \frac{1}{t^2}. \tag{0.11}$$

A similar bound is true for $D_N^{P^*}$, cf. [5]. For the cap discrepancy in [10] $D_N^C \ll \frac{1}{t}$ is established. Estimates concerning the number of points of a spherical t-design are due to Wagner [29] and Kuijlaars [16], where t-designs with

$O(t^{\frac{d(d+1)}{2}})$ points are constructed. The construction makes use of Chebyshev quadrature formulæ for ultraspherical weight functions. Delsarte, Goethals and Seidel [6] have proved that the number points of a t-design is bounded from below by

$$\begin{array}{ll} \binom{d+n-1}{d-1} + \binom{d+n-2}{d-1} & \text{for} \quad t = 2n \\ 2\binom{d+n-1}{d-1} & \text{for} \quad t = 2n+1. \end{array}$$

Bannai and Dammerell [1, 2] have shown that there exist no t-designs with equality in the above estimates.

Studying distribution properties of point sequences other quantities different from discrepancies are well known. For instance, the dispersion measures the denseness of infinite sequences. The dispersion

$$\Theta_N = \sup_{\mathbf{x}\in S^d} \min_{j\neq k} \delta(\mathbf{x}_k, \mathbf{x}) \tag{0.12}$$

(with respect to the geodesic metric δ on S^d) is just the radius of the largest spherical cap not containing one of the points $\mathbf{x}_1, \dots, \mathbf{x}_N$. Note that sequences with dispersion tending to 0 need not be uniformly distributed. This spherical cap dispersion is of great interest, because it measures the approximation error of Quasi-Monte Carlo methods for global optimization; see Niederreiter [22] and the more recent contribution [4]. A related concept is the dispersion with respect to spherical slices (i. e. intersections of two half-spheres). It is defined as the angle of the largest slice not containing one of the points $\mathbf{x}_1, \dots, \mathbf{x}_N$. This kind of dispersion is important for applications in computational geometry, cf. [25]. In [26] the following relation between dispersion and discrepancy is established:

$$\Theta_N(\mathbf{x}_n) \le c_{15}(d) \left(D_N^C\right)^{\frac{1}{d}}. \tag{0.13}$$

Furthermore, we mention another quantity for measuring the distribution behaviour of a point set $\mathbf{x}_1, \dots, \mathbf{x}_N$. For sequences in the unit cube Beardwood, Halton and Hammersley [3] studied the length $\mu_N(\mathbf{x}_n)$ of the shortest closed polygonal path joining the given points. For independently chosen random points these authors proved that

$$\mu_N \sim c_{16}(d) N^{\frac{d-1}{d}}, \quad \text{almost surely.} \tag{0.14}$$

In Section 2 of the present article we estimate $\mu_N(\mathbf{x}_n)$ from below by the spherical cap discrepancy obtaining

$$\mu_N(\mathbf{x}_n) \ge c_{17}(d) \left(D_N^C(\mathbf{x}_n)\right)^{-\frac{d-1}{d}}. \tag{0.15}$$

Finally, we remark that in principle there are several possibilities for constructing uniformly distributed sequences on the sphere. First, one can take a low-discrepancy point sequence in the unit cube and transform it via polar coordinates to the sphere. Secondly, there is a classical construction given by Pommerenke [23] using the representation of integers as sums of squares. Thirdly, Lubotzky, Phillips and Sarnak [18] established a construction using a free subgroup of the group of rotations. This methods uses a deep machinery, mainly modular forms and Hecke operators and is restricted to S^2.

1 Discrepancies Involving Pseudo-Differential Operators

In this section we want to describe a notion of discrepancy based on a certain class of pseudo-differential operators. As usual, we define the Fourier coefficient $f_{m,j}$ in the spherical harmonics expansion by

$$f_{m,j} := \int_{S^d} f(\mathbf{x}) S_{m,j}(\mathbf{x})\, d\sigma(\mathbf{x}),$$

where σ is the normalized surface measure on S^d.

We define for $s \in \mathbb{R}^+$ the *weighted Sobolev space* $H^s(\Omega)$ by

$$H^s(S^d) := \left\{ f \mid f : S^d \to \mathbb{R}, \text{ such that } \sum_{m=0}^{\infty} \sum_{j=1}^{Z(d,m)} f_{m,j}^2 \hat{m}^{2s} < \infty \right\}, \tag{1.16}$$

where

$$\hat{m} = \begin{cases} 1 & \text{if } m = 0 \\ m & \text{otherwise} \end{cases}.$$

On this space we introduce an inner product and the corresponding norm in the obvious way

$$\langle f, g \rangle_{H^s} := \sum_{m=0}^{\infty} \sum_{j=1}^{Z(d,m)} f_{m,j} g_{m,j} \hat{m}^{2s} \quad \text{and} \quad \|f\|_{H^s} := \sqrt{\sum_{m=0}^{\infty} \sum_{j=1}^{Z(d,m)} f_{m,j}^2 \hat{m}^{2s}}.$$

We proceed with an embedding theorem.

Proposition 1.2. *For $s > d/2$, $H^s(S^d)$ is a subspace of $C(S^d)$, the space of all continuous functions.*

Proof. Using the Cauchy-Schwarz inequality and the addition theorem for spherical harmonics we obtain

$$\left(\sum_{m=0}^{\infty}\sum_{j=1}^{Z(d,m)} |f_{m,j}S_{m,j}(\mathbf{x})|\right)^2 \leq$$

$$\left(\sum_{m=0}^{\infty}\sum_{j=1}^{Z(d,m)} f_{m,j}^2\hat{m}^{2s}\right)\left(\sum_{m=0}^{\infty}\sum_{j=1}^{Z(d,m)} S_{m,j}^2(\mathbf{x})\hat{m}^{-2s}\right) = \|f\|_{H^s}\sum_{m=0}^{\infty} Z(d,m)m^{-2s}.$$

Furthermore, $Z(d,m)$ satisfies

$$Z(d,m) \leq e^d m^{d-1},$$

and therefore the series (1.17) converges for $d-1-2s < -1 \iff s > d/2$. □

The key concept for our further investigations is that of a pseudo-differential operator. We call $\mathbf{T}$ a *pseudo-differential operator* on S^d with symbol $\{T_{m,j}, m = 0, 1, \ldots, 1 \leq j \leq Z(d,m)\}$ if

$$\mathbf{T}S_{m,j} = T_{m,j}\, S_{m,j}$$

holds for all spherical harmonics $S_{m,j}$. Furthermore we assume that there exist constants C_1, C_2, and s such that

$$C_1 m^s \leq T_{m,j} \leq C_2 m^s,$$

and call s the *order* of the operator $\mathbf{T}$. If $T_{m,j}$ does not depend on j, we set $T_m := T_{m,j}$.

Example 1 *Since the spherical harmonics are the eigenfunctions of the Laplace-Beltrami operator Δ corresponding to the eigenvalues $-m(m+d-1)$, we conclude that Δ is a pseudo-differential operator of order* 2.

Let $\mathbf{T}$ be any pseudo-differential operator of order s. Then we get a different representation of the space H^s by

$$H^s(S^d) = \left\{f \mid f : S^d \to \mathbb{R}, \mathbf{T}f \in \mathcal{L}_2(S^d)\right\}. \tag{1.17}$$

Now we are ready to prove an estimate for the approximation error.

Theorem 1.3. *Let* $\mathbf{T}$ *be a pseudo-differential operator of order* s *and symbol* $\{T_m\}$*, with* $s > d/2$*. Then for any function* $f \in H^s$ *we have*

$$E_N(f) \le \frac{1}{N}\sqrt{\sum_{i=0}^{N}\sum_{\ell=0}^{N}\sum_{m=1}^{\infty}\frac{Z(d,m)}{T_m^2}P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell\rangle)}\ \|Tf\|_{H^s}.$$

Proof. It is well known that the spherical harmonic expansion

$$f(\mathbf{x}) = \sum_{m=0}^{\infty}\sum_{j=1}^{Z(d,m)} f_{m,j}S_{m,j}(\mathbf{x})$$

converges uniformly since we have demanded $s > d/2$. Now we apply $\mathbf{T}$ to the above series, multiply by $S_{m,j}$ and integrate over S^d to obtain

$$f_{m,j} = \int_{S^d}\frac{\mathbf{T}f(\mathbf{y})S_{m,j}(\mathbf{y})}{T_m}\,d\sigma(\mathbf{y}),\ \text{for } m > 1.$$

This means we can rewrite the spherical harmonic expansion

$$f(\mathbf{x}) = \int_{S^d} f(\mathbf{y})\,d\sigma(\mathbf{y}) + \sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\int_{S^d}\frac{\mathbf{T}f(\mathbf{y})S_{m,j}(\mathbf{y})}{T_m}\,d\sigma(\mathbf{y})\,S_{m,j}(\mathbf{x}).$$

If we put $\mathbf{x} = \mathbf{x}_n$ and sum over n, we get

$$\begin{aligned}\frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x}_n) &= \int_{S^d} f(\mathbf{x})\,d\sigma(\mathbf{x}) \\ &\quad + \sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\int_{S^d}\frac{\mathbf{T}f(\mathbf{y})S_{m,j}(\mathbf{y})}{T_m}\,d\sigma(\mathbf{y})\,\frac{1}{N}\left(\sum_{n=1}^{N} S_{m,j}(\mathbf{x}_n)\right).\end{aligned}$$

Clearly, the approximation error can be estimated by the absolute value of the last term in (1.18):

$$E_N(f) \ \le\ \frac{1}{N}\left|\int_{S^d}\mathbf{T}f(\mathbf{y})\sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\sum_{n=1}^{N}\frac{S_{m,j}(\mathbf{x}_n)S_{m,j}(\mathbf{y})}{T_m}\,d\sigma(\mathbf{y})\right|$$

$$
\begin{aligned}
&\leq \frac{1}{N}\left(\int_{S^d}(\mathbf{T}f(\mathbf{y}))^2\,d\sigma(\mathbf{y})\right)^{\frac{1}{2}} \times \\
&\qquad \times\left[\int_{S^d}\left(\sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\sum_{n=1}^{N}\frac{S_{m,j}(\mathbf{x}_n)S_{m,j}(\mathbf{y})}{T_m}\right)^2 d\sigma(\mathbf{y})\right]^{\frac{1}{2}} \\
&\leq \frac{1}{N}\|\mathbf{T}f\|_2\left[\sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\frac{1}{T_{m,j}^2}\left(\sum_{n=1}^{N}S_{m,j}(\mathbf{x}_n)\right)^2\right]^{\frac{1}{2}} \\
&\leq \frac{1}{N}\|\mathbf{T}f\|_2\left[\sum_{i=1}^{N}\sum_{\ell=1}^{N}\sum_{m=1}^{\infty}\sum_{j=1}^{Z(d,m)}\frac{1}{T_{m,j}^2}S_{m,j}(\mathbf{x}_i)\,S_{m,j}(\mathbf{x}_\ell)\right]^{\frac{1}{2}} \\
&\leq \frac{1}{N}\|\mathbf{T}f\|_2\left[\sum_{i=1}^{N}\sum_{\ell=1}^{N}\sum_{m=1}^{\infty}\frac{Z(d,m)}{T_m^2}P_m^d(\langle\mathbf{x}_i,\mathbf{x}_\ell\rangle)\right]^{\frac{1}{2}},
\end{aligned}
$$

where we have used the Cauchy-Schwarz inequality, the orthonormality of $S_{m,j}$ and the addition theorem. Since by (1.17) $\|\mathbf{T}\cdot\|_2 = \|\cdot\|_{H^s}$ we have completed the proof. □

The first factor in the estimate for the error is independent of the function and depends only on the point set. Therefore we can introduce a discrepancy by

$$
D_N(\mathbf{x}_n;\mathbf{T}) := \frac{1}{N}\left[\sum_{i=1}^{N}\sum_{\ell=1}^{N}\sum_{m=1}^{\infty}\frac{Z(d,m)}{T_m^2}P_m^d(\langle\mathbf{x}_i,\mathbf{x}_\ell\rangle)\right]^{\frac{1}{2}}. \tag{1.18}
$$

Since $Z(d,m) \ll m^{d-1}$ and $T_m^2 \gg m^{2s}$ with $s > \frac{d}{2}$, this quantity is bounded for $N \to \infty$.

Theorem 1.4. *Let $f \in H^s$, where $s > d + \frac{1}{2}$. Then*

$$
E_N(f) \leq c_s\,\|f\|_{H^s} D_N^C(\mathbf{x}_n).
$$

Proof. Let $\mathbf{T}$ be a pseudo-differential operator of order s. By the result of Theorem 1.3 it suffices to show that

$$
D_N(\mathbf{x}_n;\mathbf{T}) \ll D_N^C(\mathbf{x}_n).
$$

Now

$$D_N(\mathbf{x}_n;\mathbf{T}) \le \sum_{m=1}^{\infty} \frac{Z(d,m)\, m^d}{T_m^2}\, D_N^P(\mathbf{x}_n). \tag{1.19}$$

Since $D_N^P(\mathbf{x}_n) \ll D_N^C(\mathbf{x}_n)$, we are finished once we have shown that the series (1.19) converges. But as $\mathbf{T}$ is of order s we have

$$T_m \ll m^s,$$

and the series (1.19) is bounded by

$$c_{18}(d) D_N^P(\mathbf{x}_n) \sum_{m=1}^{\infty} m^{2d}\, m^{-2s},$$

which is finite if $2d - 2s < -1 \iff s > d + \frac{1}{2}$. □

A specialisation of the pseudo-differential operator leads to the discrepancy $D_N^{P^*}$, which was defined in the introduction for $d = 2$. Consider the operator $\mathbf{A}$ for S^2 with symbol $A_m^2 = (2m+1)m(m+1)$. Now the identity

$$\sum_{n=1}^{\infty} \frac{P_m^2(t)}{m(m+1)} = 1 - 2\ln\left(1 + \sqrt{\frac{1-t}{2}}\right)$$

together with formula (1.18) yields immediately

$$D_N(\mathbf{x}_n;\mathbf{A}) = D_N^{P^*}(\mathbf{x}_n).$$

We will now generalize this idea to arbitrary dimensions. To evaluate the sum in (1.18) we will use the generating functions of the Legendre polynomials (0.5). Consider the operator $\mathbf{A}$ for S^d with the symbol

$$A_m^2 = Z(d,m)m(m+d-1),$$

which together with formula (1.18) suggests the following definition

$$D_N^{P^*}(\mathbf{x}_n) := D_N(\mathbf{x}_n;\mathbf{A}) = \frac{1}{N}\left[\sum_{i=1}^{N}\sum_{\ell=1}^{N}\sum_{m=1}^{\infty} \frac{1}{m(m+d-1)} P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell\rangle)\right]^{\frac{1}{2}}. \tag{1.20}$$

Theorem 1.5.

$$D_N^P(\mathbf{x}_n) \le D_N^{P^*}(\mathbf{x}_n) \le c_{14}(d)\left(D_N^P\right)^{\frac{1}{2(d+1)}}.$$

Proof. The left hand side inequality is obvious. For the proof of the right hand side choose $K = [(D_N^P)^{-\frac{1}{2(d+1)}}]$ and estimate

$$\begin{aligned}
\left(D_N^{P^*}\right)^2 &= \sum_{m=1}^{\infty} \frac{m^{2d}}{m(m+d-1)} \frac{1}{m^{2d}} \frac{1}{N^2} \sum_{i=1}^{N} \sum_{\ell=1}^{N} P_m^d(\langle \mathbf{x}_i, \mathbf{x}_\ell \rangle) \\
&\le \sum_{m=1}^{K} \frac{m^{2d-1}}{m+d-1} \left(D_N^P\right)^2 + \sum_{m=K+1}^{\infty} \frac{1}{m(m+d-1)} \\
&\ll K^{2d-1} \left(D_N^P\right)^2 + \frac{1}{K} \ll \left(D_N^P\right)^{\frac{1}{d+1}},
\end{aligned}$$

which proves the theorem. □

The following proposition shows how we can use generating functions to evaluate the series (1.20). We omit a detailed proof which runs by induction.

Proposition 1.6. *Let* $\ell \ge 0,\ k \ge 0$ *and*

$$g(\omega) = \sum_{m=1}^{\infty} c_m \omega^m.$$

Then

$$\sum_{m=1}^{\infty} \frac{c_m \omega^m}{(m+\ell)(m+\ell+1)\cdots(m+\ell+k)} = \frac{1}{k!} \sum_{i=0}^{k} (-1)^i \binom{k}{i} \frac{1}{\omega^{\ell+i}} \int_0^{\omega} g(y) y^{\ell+i-1} dy. \tag{1.21}$$

Corollary 1.7.

$$\sum_{m=1}^{\infty} \frac{P_m^d(x)}{m(m+d-1)} = \int_0^1 \left((y^2 - 2yx + 1)^{-\frac{d-1}{2}} - 1\right) \frac{(1-y)^{d-1}}{y}\, dy.$$

Proof. We again use generating functions. Set $\ell = 0$, $k = d-1$,

$$c_m = (m+1)(m+2)\cdots(m+d-2) P_m^d(x),$$

and

$$g(\omega) = \frac{1}{(1 - 2x\omega + \omega^2)^{(d-1)/2}} - 1$$

in the proposition and the result follows setting $\omega = 1$. □

The integrals, which appear in (1.21), can be evaluated using the formula

$$\begin{aligned} \int \frac{x^m}{(ax^2+c)^{k+1/2}}\,dx &= \frac{1}{(2k-1)c}\frac{x^{m+1}}{(ax^2+c)^{k-1/2}} \\ &+ \frac{2k-m-2}{(2k-1)c}\int \frac{x^m}{(ax^2+c)^{k-1/2}}\,dx, \end{aligned}$$

cf. [11], page 43. It is therefore clear that the expression on the right hand side in (1.21) can be expressed by elementary functions. We will use the program MAPLE to compute this expression for the case $d = 3$ and obtain

$$\frac{3}{2} - 2\sqrt{\frac{1-x}{1+x}}\arctan\sqrt{\frac{1+x}{1-x}} =: \psi(x)$$

for the right hand side in Corollary 1.7.

Thus we have for $d = 3$

$$D_N^{P^*}(\mathbf{x}_n) = \frac{1}{N}\left(\sum_{i=1}^{N}\sum_{\ell=1}^{N}\psi(\langle \mathbf{x}_i, \mathbf{x}_\ell\rangle)\right)^{\frac{1}{2}}.$$

2 Shortest Paths on the Sphere

In this section we will estimate the length of the shortest path through a point set on the sphere S^d in terms of the spherical cap discrepancy.

The following result is due to Wyner [30](p. 1090).

Proposition 2.8. *The maximal number $M(\rho)$ of non-intersecting spherical caps with radius ρ satisfies*

$$M(\rho) \geq \frac{\omega_d}{A(2\rho)},$$

where $A(\rho)$ is the surface area of a cap with radius ρ and ω_d denotes the surface area of S^d.

Proof. Let $\{C(\mathbf{x}_1,\rho),\dots,C(\mathbf{x}_{M(\rho)},\rho)\}$ be a maximal set of non-intersecting caps. Then the set $\{C(\mathbf{x}_1,2\rho),\dots,C(\mathbf{x}_{M(\rho)},2\rho)\}$ covers the whole sphere, since

$$\mathbf{y}\notin\bigcup_{n=1}^{M(\rho)}C(\mathbf{x}_n,2\rho)$$

implies that $C(\mathbf{y},\rho)$ would not intersect any of the $C(\mathbf{x}_n,\rho)$. Therefore

$$M(\rho)\,A(2\rho)\geq\omega_d,$$

which proves the proposition. □

Theorem 2.9. *Let $\mathbf{x}_1,\mathbf{x}_2,\dots$ be a point sequence on S^d. Then for sufficiently large N*

$$\mu(N)\geq c_{17}(d)\,\left(D_N^C(\mathbf{x}_n)\right)^{-(d-1)/d},$$

where $c_{17}(d)$ only depends on the dimension d.

Proof. From [30](p. 1090) we know

$$A(\rho)=\frac{d\,\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}\int_0^\rho(\sin\phi)^{d-1}\,d\phi=:\kappa_d\int_0^\rho(\sin\phi)^{d-1}\,d\phi. \tag{2.22}$$

Now choose ρ such that

$$D_N^C(\mathbf{x}_n)=A(\alpha\rho), \tag{2.23}$$

where α is some for the moment arbitrary constant in the interval $(0,1)$. This is possible for large enough N since $A(\rho)$ is a continuous strictly increasing function. From Proposition 2.8 it follows that we can place $M(\rho)\geq\frac{\omega_d}{A(2\rho)}$ non-intersecting caps with angle ρ on S^d. Now we conclude to obtain

$$\mu_N(\mathbf{x}_n)\geq(1-\alpha)2\rho M(\rho)\geq(1-\alpha)2\rho\frac{\omega_d}{A(2\rho)}.$$

From (2.22) and $\sin x\leq x$ we get

$$\mu(N)\geq c_{19}(d)(1-\alpha)\rho^{1-d}.$$

On the other hand (2.23) and the fact that $\sin x\geq\frac{2}{\pi}x$ for $x\in[0,\frac{\pi}{2}]$ yield

$$D_N^C(\mathbf{x}_n)\leq c_{20}(d)\,\alpha^d\rho^d$$

Combining these two results we obtain

$$\begin{aligned} \mu_N(\mathbf{x}_n) &\geq c_{19}(d)(1-\alpha)\left[\left(\frac{D_N^C(\mathbf{x}_n)}{c_{20}(d)}\right)^{\frac{1}{d}} \alpha^{-1}\right]^{-(d-1)} \\ &= c_{19}(d)\left(c_{20}(d)\right)^{\frac{d-1}{d}} \left(\alpha^{d-1}-\alpha^d\right) \left(D_N^C(\mathbf{x}_n)\right)^{-\frac{d-1}{d}}, \end{aligned}$$

where the optimal constant is attained for $\alpha = (d-1)/d$. □

Remark 2 *We note that for a suitable infinite sequence of points* $(\mathbf{x}_n)$ *contained in one half sphere,* $\mu_N(\mathbf{x}_n)$ *may tend to infinity, whereas* $D_N^C(\mathbf{x}_n) \geq \frac{1}{2}$ *(for all* N*). This means that there are no upper bounds for* $\mu_N(\mathbf{x}_n)$ *of the same shape as the lower bound (0.15).*

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