

EQUIDISTRIBUTION ON THE SPHERE*

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Abstract. A concept of generalized discrepancy, which involves pseudodifferential operators to give a criterion of equidistributed pointsets, is developed on the sphere. A simply structured formula in terms of elementary functions is established for the computation of the generalized discrepancy. With the help of this formula five kinds of point systems on the sphere, namely lattices in polar coordinates, transformed two-dimensional sequences, rotations on the sphere, triangulations, and “sum of three squares sequence,” are investigated. Quantitative tests are done, and the results are compared with one another. Our calculations exhibit different orders of convergence of the generalized discrepancy for different types of point systems.

Key words. sphere, pointsets, pseudodifferential operators, generalized discrepancy, equidistribution, low discrepancy (quasi-Monte-Carlo) method, approximate integration

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1. Introduction. Of practical importance is the problem of generating equidistributed pointsets on the sphere. For that reason the concept of generalized discrepancy, which involves pseudodifferential operators to give a quantifying criterion of equidistributed pointsets, is of great interest. In this paper an explicit formula in terms of elementary functions is developed for the generalized discrepancy. Essential tools are Sobolev space structures and pseudodifferential operator techniques. It is mentioned that an optimal pointset may be obtained by minimizing the generalized discrepancy. But, in spite of the elementary representation of the generalized discrepancy, this is a nonlinear optimization problem which will not be discussed here. Our investigations, however, show that there are many promising ways to generate point systems on the sphere such that the discrepancy becomes small. To be specific, we distinguish five kinds of point systems on the sphere: lattices in polar coordinates, transformed two-dimensional sequences, rotations on the sphere, triangulations, and “sum of three squares sequence.” By using our developed formulas, the five classes of point systems are described, and their discrepancies are explicitly calculated for increasing numbers of points. The results show different orders of convergence indicated by the generalized discrepancy. Furthermore, our computations enable us to give a quantitative comparison between the different point systems. It is somewhat surprising that certain types of transformed sequences yield the best results. Nevertheless, there are special other pointsets which provide us with better results for comparable numbers of points. For instance, the soccer ball (C_{60}) leads us to the best result in all our considered pointsets of about 60 points.

The problem of generating a large number of “equidistributed points” on the sphere has many applications in various fields of computation, particularly in geoscience and medicine. The advantage of equidistributed point systems lies in the fact that relatively few samplings of the data are needed, and approximate integration can be simply performed by computation of a mean value, i.e., the arithmetical mean.

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The outline of the paper is as follows: section 2 begins with a discussion of Sobolev spaces and (invariant) pseudodifferential operators on the sphere. The generalized discrepancy is developed in section 3. The announced point systems are studied in section 4. The low discrepancy method, also called the quasi-Monte-Carlo method, for numerical integration on the sphere is discussed in section 5 for three types of test examples.

2. Sobolev spaces and pseudodifferential operators on the sphere. Let \mathbb{R}^3 denote the three-dimensional Euclidean space. We use $x, y, z \dots$ to represent the elements of \mathbb{R}^3 and the Greek alphabet $\xi, \eta \dots$ to represent the vectors of the unit sphere Ω in \mathbb{R}^3 . Δ^* denotes the Beltrami operator on the unit sphere. A function $F : \Omega \mapsto \mathbb{R}$ possessing k continuous derivatives on Ω is said to be of the class $C^k(\Omega)$. $C(\Omega) = C^0(\Omega)$ is the class of real continuous scalar-valued functions on Ω . By $L^2(\Omega)$ we denote the space of Lebesgue square-integrable scalar functions on Ω . The spherical harmonics of degree n are defined as the everywhere on Ω infinitely differentiable eigenfunctions of the Beltrami operator Δ^* corresponding to the eigenvalues $(\Delta^*)_n = -n(n+1)$, $n = 0, 1, \dots$. As it is well known (cf., e.g., [14]), the linear space $Harm_n$ of all spherical harmonics of degree n is of dimension $2n+1$. We denote $\{Y_{n,j}; n = 0, 1, \dots; j = 1, 2, \dots, 2n+1\}$ to be an orthonormalized basis of $L^2(\Omega)$, where n is called degree and j is the order of the spherical harmonics. The space $Harm_{0,\dots,m}$ of all spherical harmonics of degree $\leq m$ possesses the dimension $(m+1)^2$. The Legendre polynomials P_n are the infinitely differentiable eigenfunctions of the Legendre operator satisfying the normalization condition $P_n(1) = 1$. It should be noted that $|P_n(t)| \leq 1$ and $|P'_n(t)| \leq \frac{n(n+1)}{2}$ for all $t \in [-1, +1]$ and all $n \in \mathbb{N}_0$. The well-known addition theorem of spherical harmonics states (cf. [5], [14])

$$(1) \quad \sum_{j=1}^{2n+1} Y_{n,j}(\xi) Y_{n,j}(\eta) = \frac{2n+1}{4\pi} P_n(\xi \cdot \eta), (\xi, \eta) \in \Omega \times \Omega.$$

In particular, we have

$$(2) \quad \sum_{j=1}^{2n+1} |Y_{n,j}(\xi)|^2 = \frac{2n+1}{4\pi}, \quad |Y_{n,j}(\xi)| \leq \sqrt{\frac{2n+1}{4\pi}}, \xi \in \Omega.$$

For $s \in \mathbb{R}$ consider the space

$$(3) \quad E^s(\Omega) = \left\{ F \in C^\infty(\Omega) \mid \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} F_{n,j}^2 \hat{n}^{2s} < \infty \right\},$$

where $F_{n,j}$ are the spherical harmonic coefficients of F and, by definition,

$$(4) \quad \hat{n} = \begin{cases} 1 & \text{if } n = 0, \\ n & \text{elsewhere.} \end{cases}$$

We are able to impose an inner product on $E^s(\Omega)$ as follows:

$$(5) \quad \langle F, G \rangle_{H^s} = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} F_{n,j} G_{n,j} \hat{n}^{2s}.$$

The Sobolev space $H^s(\Omega)$ is the completion of $E^s(\Omega)$ with respect to the topology $\|\cdot\|_{H^s} = (\cdot, \cdot)_{H^s}^{\frac{1}{2}}$. The following relationships between Sobolev spaces are valid:

$H^{s_1}(\Omega) \subset H^{s_2}(\Omega)$, whenever $s_1 > s_2$. Sobolev spaces and classical function spaces $C^k(\Omega)$ are related via imbedding theorems.

LEMMA 2.1 (imbedding theorem). $H^s(\Omega)$ is a subspace of $C^k(\Omega)$ if $s > k + 1$.

Proof. It is sufficient to prove Lemma 2.1 for the case $k = 0$. For $s > 1$, applying the Cauchy–Schwarz inequality we obtain

$$\sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} |F_{n,j} Y_{n,j}(\xi)| \leq \left(\sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} F_{n,j}^2 \hat{n}^{2s} \right)^{\frac{1}{2}} \left(\sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} (Y_{n,j}(\xi))^2 \hat{n}^{-2s} \right)^{\frac{1}{2}}.$$

From the addition theorem of the spherical harmonics it follows that

$$C = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} (Y_{n,j}(\xi))^2 \hat{n}^{-2s} = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi \hat{n}^{2s}} < \infty,$$

provided that $s > 1$. Therefore, the series is absolutely and uniformly convergent. But this means that F corresponds to a continuous function on Ω . \square

From Lemma 2.1 (imbedding theorem) we are able to conclude that the spherical harmonic expansion of any function in $H^s(\Omega)$ converges uniformly provided that $s > 1$. This is significant because there are functions in $C(\Omega)$ which do not allow a uniformly convergent spherical harmonic expansion (cf. [7]).

With the aid of the Sobolev space structure introduced above we make some comments on (invariant) pseudodifferential operators on the sphere, since these operators do not belong to the traditional equipment.

DEFINITION 2.1 (pseudodifferential operator on the sphere). Let $\{A_n\}, n = 0, 1, \dots$, be a sequence of real numbers A_n satisfying

$$\lim_{n \rightarrow \infty} \frac{|A_n|}{(n + \frac{1}{2})^t} = \text{const} \neq 0$$

for some $t \in \mathbb{R}$. Then the operator $\mathbf{A} : H^s(\Omega) \mapsto H^{s-t}(\Omega)$ defined by

$$(6) \quad \mathbf{A}F = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} A_n F_{n,j} Y_{n,j}, F \in H^s(\Omega)$$

is called the pseudodifferential operator of order t . $\{A_n\}$ is called the spherical symbol of \mathbf{A} . Moreover, if

$$\lim_{n \rightarrow \infty} \frac{|A_n|}{(n + \frac{1}{2})^t} = 0$$

for all $t \in \mathbb{R}$, then the operator $\mathbf{A} : H^s(\Omega) \mapsto C^\infty(\Omega)$ is called the pseudodifferential operator of order $-\infty$ (note that equation (6) is understood in $H^{s-t}(\Omega)$ -topology).

The spherical symbol has many appealing properties. For example, it is readily seen that $(\mathbf{A}' + \mathbf{A}'')_n = A'_n + A''_n, (\mathbf{A}'\mathbf{A}'')_n = A'_n A''_n$ for every choice of pseudodifferential operators $\mathbf{A}', \mathbf{A}''$. Obviously we have

$$\mathbf{A}Y_{n,j} = A_n Y_{n,j}, \quad n = 0, 1, \dots, j = 1, \dots, n+1$$

(i.e., all pseudodifferential operators considered here are invariant operators). Using the kernel

$$K_{\mathbf{A}}(\xi \cdot \eta) = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} A_n Y_{n,j}(\xi) Y_{n,j}(\eta) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} A_n P_n(\xi \cdot \eta),$$

we obtain $\mathbf{A}F$ by convolution as follows:

$$\mathbf{A}F = K_{\mathbf{A}} * F = \int_{\Omega} K_{\mathbf{A}}(\cdot\eta)F(\eta)d\omega(\eta).$$

The kernel satisfies the property $K_{\mathbf{A}} \in H^{-(t+\epsilon)}(\Omega)$ for all $\epsilon > 0$ provided that $t > -\infty$. In the case $t = -\infty$ we have $K_{\mathbf{A}} \in C^\infty(\Omega)$.

In what follows we list some particularly important pseudodifferential operators:

(1) The Beltrami operator Δ^* is not invertible, since $(\Delta^*)_n = 0$ for $n = 0$, but the operator $-\Delta^* + \frac{1}{4}$ has the symbol $\{(n + \frac{1}{2})^2\}$, $n = 0, 1, \dots$, and, hence, has an inverse $(-\Delta^* + \frac{1}{4})^{-1}$ which is a pseudodifferential operator of order -2 . More generally, $(-\Delta^* + \frac{1}{4})^s$ is a pseudodifferential operator of order $2s$ and has the spherical symbol $\{(n + \frac{1}{2})^{2s}\}$, $n = 0, 1, \dots$. Using the kernel $K_{(-\Delta^* + \frac{1}{4})^{-2s}}$, $s > 1$, we obtain

$$F(\xi) = \int_{\Omega} \left(-\Delta^* + \frac{1}{4}\right)^s K_{(-\Delta^* + \frac{1}{4})^{-2s}}(\xi \cdot \eta) \left(-\Delta^* + \frac{1}{4}\right)^s F(\eta) d\omega(\eta)$$

for all $F \in H^s(\Omega)$ and $\xi \in \Omega$. This is easily seen by the Parseval identity for the system of $\mathcal{L}^2(\Omega)$ - orthonormal spherical harmonics.

(2) The integral operator of the single layer potential on Ω given by

$$(7) \quad \mathbf{A}U(\xi) = \frac{1}{2\pi} \int_{\Omega} \frac{U(\eta)}{|\xi - \eta|} d\omega(\eta), \xi \in \Omega,$$

is a pseudodifferential operator of order -1 possessing the symbol $\{A_n\}$ with $A_n = (n + \frac{1}{2})^{-1}$. This can be seen by inserting the expansion of $|\xi - \eta|^{-1}$ in terms of Legendre polynomials. A consequence is that \mathbf{A} is invertible. Other types of geodetically relevant integral operators can be found in [17].

(3) The operator $\mathbf{A} = (-2\Delta^*)(-\Delta^* + \frac{1}{4})^{\frac{1}{2}}$ has the symbol $\{A_n\}$, where A_n is given by $A_n = (2n+1)n(n+1)$, $n = 0, 1, \dots$. \mathbf{A} is not invertible, but the related operator \mathbf{B} with symbol $\{B_n\}$ given by

$$B_n = \begin{cases} 1, & n = 0, \\ (2n+1)(n(n+1)), & n = 1, 2, \dots \end{cases}$$

is invertible. Since (cf., e.g., [12])

$$\sum_{n=1}^{\infty} \frac{1}{n(n+1)} P_n(t) = 1 - 2 \ln \left(1 + \sqrt{\frac{1-t}{2}} \right), \quad t \in [-1, +1]$$

we find

$$K_{\mathbf{B}^{-1}}(\xi \cdot \eta) = \frac{1}{2\pi} - \frac{1}{2\pi} \ln \left(1 + \sqrt{\frac{1 - \xi \cdot \eta}{2}} \right)$$

for all $\xi, \eta \in \Omega$.

(4) $A_n = r^n$, $0 \leq r < 1$ (or $A_n = e^{\frac{1}{2}n(n+1)h}$, $h > 0$) define pseudodifferential operators of order $-\infty$.

To show the relationship between the pseudodifferential operators and the Sobolev spaces we give an equivalent reformulation of the Sobolev space $H^s(\Omega)$. Let \mathbf{A} be a pseudodifferential operator of order s . Then, the Sobolev space $H^s(\Omega)$ can be equivalently expressed in the following form:

$$(8) \quad H^s(\Omega) = \{F|F : \Omega \mapsto \mathbb{R}, \quad \mathbf{A}F \in L^2(\Omega)\}.$$

3. Equidistribution on the sphere. In this section we discuss the problem of equidistribution. This problem can be stated as follows: find a pointset $\{\eta_1, \dots, \eta_N\}$ such that the remainder term

$$(9) \quad \left| \int_{\Omega} G(\xi) d\omega(\xi) - \frac{4\pi}{N} \sum_{i=1}^N G(\eta_i) \right|$$

for any function $G \in H^s(\Omega)$ converges to 0 as $N \rightarrow \infty$.

Let us begin the discussion with an a priori estimate of the remainder. The result is an analogue to the Koksma–Hlawka inequality in Euclidean spaces (see also, [8, 9, 10] and many other references therein).

THEOREM 3.1. *Let \mathbf{A} be a pseudodifferential operator of order s , $s > 1$, with the symbol $\{A_n\}$ satisfying $A_n \neq 0, n \geq 1$. Then, for any function $\mathbf{A}G \in L^2(\Omega)$, we have the estimate*

$$(10) \quad \left| \frac{1}{4\pi} \int_{\Omega} G(\xi) d\omega(\xi) - \frac{1}{N} \sum_{i=1}^N G(\eta_i) \right| \leq \frac{1}{N} \left[\sum_{t=1}^N \sum_{i=1}^N \sum_{n=1}^{\infty} \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}} \|\mathbf{A}G\|_{L^2}.$$

Proof. From (8) we know that $\mathbf{A}G \in L^2(\Omega)$ is equivalent to $G \in H^s(\Omega)$. Because of the assumption $s > 1$ it follows from Lemma 2.1 (imbedding theorem) that the spherical harmonic expansion

$$G(\xi) = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} G_{n,j} Y_{n,j}(\xi), \xi \in \Omega$$

converges absolutely and uniformly. We rewrite the spherical harmonic expansion of G as follows:

$$G(\xi) = \frac{1}{4\pi} \int_{\Omega} G(\eta) d\omega(\eta) + \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \int_{\Omega} \frac{\mathbf{A}G(\eta) Y_{n,j}(\eta)}{A_n} d\omega(\eta) Y_{n,j}(\xi).$$

By setting $\xi = \eta_i$ and taking the sum over all indices $i, 1 \leq i \leq N$, we obtain

$$\frac{1}{N} \sum_{i=1}^N G(\eta_i) = \frac{1}{4\pi} \int_{\Omega} G(\eta) d\omega(\eta) + \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \int_{\Omega} \frac{\mathbf{A}G(\eta) Y_{n,j}(\eta)}{A_n} d\omega(\eta) \left[\frac{1}{N} \sum_{i=1}^N Y_{n,j}(\eta_i) \right].$$

Hence, the integral error can then be estimated as follows:

$$\begin{aligned} & \left| \frac{1}{4\pi} \int_{\Omega} G(\eta) d\omega(\eta) - \frac{1}{N} \sum_{i=1}^N G(\eta_i) \right| \\ & \leq \left| \frac{1}{N} \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \sum_{i=1}^N \frac{Y_{n,j}(\eta_i)}{A_n} \int_{\Omega} \mathbf{A}G(\eta) Y_{n,j}(\eta) d\omega(\eta) \right| \\ & = \left| \frac{1}{N} \int_{\Omega} \mathbf{A}G(\eta) \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \sum_{i=1}^N \frac{Y_{n,j}(\eta_i) Y_{n,j}(\eta)}{A_n} d\omega(\eta) \right|. \end{aligned}$$

By using the Cauchy–Schwarz inequality and the addition theorem of the spherical harmonics we get

$$\begin{aligned}
& \left| \frac{1}{4\pi} \int_{\Omega} G(\eta) d\omega(\eta) - \frac{1}{N} \sum_{i=1}^N G(\eta_i) \right| \\
& \leq \frac{1}{N} \left[\int_{\Omega} (\mathbf{A}G(\eta))^2 d\omega(\eta) \right]^{\frac{1}{2}} \left[\int_{\Omega} \left(\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \sum_{i=1}^N \frac{Y_{n,j}(\eta_i) Y_{n,j}(\eta)}{A_n} \right)^2 d\omega(\eta) \right]^{\frac{1}{2}} \\
& = \frac{1}{N} \|\mathbf{A}G\|_{L^2} \left[\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \left(\frac{\sum_{i=1}^N Y_{n,j}(\eta_i)}{A_n} \right)^2 \right]^{\frac{1}{2}} \\
& = \frac{1}{N} \|\mathbf{A}G\|_{L^2} \left[\sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \frac{Y_{n,j}(\eta_i) Y_{n,j}(\eta_t)}{A_n^2} \right]^{\frac{1}{2}} \\
& = \frac{1}{N} \|\mathbf{A}G\|_{L^2} \left[\sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}}.
\end{aligned}$$

This completes the proof. \square

Theorem 3.1 extends a result given for the Beltrami operator (cf. [5]) to the general context of pseudodifferential operators. It is obvious that the right-hand side of the estimate (10) consists of two parts. The first part depends only on the pointset, while the second part depends merely on the function G under consideration. This gives rise to the definition of generalized discrepancy.

DEFINITION 3.1 (generalized discrepancy). *Let \mathbf{A} be a pseudodifferential operator of order s , $s > 1$, with symbol $\{A_n\}$, $A_n \neq 0$ for $n \geq 1$. Then the generalized discrepancy associated with a pseudodifferential operator \mathbf{A} is defined by*

$$(11) \quad D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) = \frac{1}{N} \left[\sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}}.$$

The generalized discrepancy characterizes “how well a pointset is equidistributed.” This can be explained by a heuristic geometrical interpretation as follows: for any subset B of Ω and any pointset $\{\eta_1, \dots, \eta_N\}$ on Ω we define the counting function

$$(12) \quad \#B = \sum_{i=1}^N \chi_B(\eta_i),$$

where χ_B is the characteristic function of B . Thus $\#B$ indicates the number n , $1 \leq n \leq N$ of points η_i contained in B . Let $\chi_B^\epsilon \in H^s$, $s > 1$ be a “smooth” approximation of the characteristic function χ_B . Then, for any nonempty Lebesgue-measurable subset B of Ω , we have an integral inequality of the following form:

$$\begin{aligned}
(13) \quad & \left| \frac{\#B}{N} - \frac{1}{4\pi} \int_{\Omega} \chi_B d\omega(\xi) \right| = \left| \frac{1}{N} \sum_{i=1}^N \chi_B(\eta_i) - \frac{1}{4\pi} \int_{\Omega} \chi_B d\omega(\xi) \right| \\
& \approx \left| \frac{1}{N} \sum_{i=1}^N \chi_B^\epsilon(\eta_i) - \frac{1}{4\pi} \int_{\Omega} \chi_B^\epsilon d\omega(\xi) \right| \leq D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) \|\mathbf{A}\chi_B^\epsilon\|_{L^2}.
\end{aligned}$$

Therefore, the generalized discrepancy gives a quantitative description of how well a pointset is equidistributed.

Remark. It is also worthwhile to translate the Wozniakowski idea of averaging the integration error (cf. [13]) into the spherical context. But this is a challenge for future work.

For different pseudodifferential operators we have different generalized discrepancies. It is of interest to understand the relationship between different generalized discrepancies associated with different pseudodifferential operators.

LEMMA 3.1. *Let \mathbf{A} , \mathbf{B} be two pseudodifferential operators of order s_1 , s_2 ($s_1 > 1$, $s_2 > 1$), and with symbols $\{A_n\}$, $\{B_n\}$ satisfying $A_n \neq 0, B_n \neq 0$ for $n \geq 1$, respectively. Then the following relations are valid for the generalized discrepancies associated with the pseudodifferential operators \mathbf{A} and \mathbf{B} :*

(1) *If the two pseudodifferential operators \mathbf{A} and \mathbf{B} are of the same order, i.e., $s_1 = s_2$, then there exist two positive constants C_1 and C_2 such that*

$$(14) \quad C_1 D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) \leq D(\{\eta_1, \dots, \eta_N\}; \mathbf{B}) \leq C_2 D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}).$$

(2) *If $s_1 > s_2$, then there exists a constant C_3 such that*

$$(15) \quad D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) < C_3 D(\{\eta_1, \dots, \eta_N\}; \mathbf{B}).$$

Proof. Applying the addition theorem of spherical harmonics we have

$$\begin{aligned} \sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) &= \sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \frac{Y_{n,j}(\eta_i) Y_{n,j}(\eta_t)}{A_n^2} \\ &= \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \left(\frac{\sum_{i=1}^N Y_{n,j}(\eta_i)}{A_n} \right)^2. \end{aligned}$$

Thus the generalized discrepancy can be rewritten as follows:

$$D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) = \left[\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \left(\frac{\sum_{i=1}^N Y_{n,j}(\eta_i)}{A_n} \right)^2 \right]^{\frac{1}{2}}.$$

If $s_1 = s_2$, then it follows from our definition of pseudodifferential operators that there exist two constants C_1 and C_2 such that

$$C_1 \left(\frac{1}{A_n} \right)^2 \leq \left(\frac{1}{B_n} \right)^2 \leq C_2 \left(\frac{1}{A_n} \right)^2, n \geq 1.$$

Therefore, it is clear that

$$C_1 D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) \leq D(\{\eta_1, \dots, \eta_N\}; \mathbf{B}) \leq C_2 D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}).$$

Part 2 can be proved in the same manner. \square

From Lemma 3.1 we deduce that the generalized discrepancy is dependent only on the order of the pseudodifferential operators. Using the generalized discrepancy we can study the property of point systems in a quantitative way.

DEFINITION 3.2 (equidistribution in $H^s(\Omega)$). *A point system $\{\eta_1^N, \dots, \eta_N^N\}$, $N = 1, 2, \dots$ is called \mathbf{A} -equidistributed in $H^s(\Omega)$, $s > 1$ if the generalized discrepancy associated with a pseudodifferential operator \mathbf{A} of order s , $s > 1$ satisfies*

$$(16) \quad \lim_{N \rightarrow \infty} D(\{\eta_1^N, \dots, \eta_N^N\}; \mathbf{A}) = 0.$$

It should be noted that if a point system is equidistributed in $H^{s_0}(\Omega)$, $s_0 > 1$, then the point system is equidistributed in $H^s(\Omega)$, $s > s_0$. This shows us that we should use s_0 , $s_0 > 1$ as small as possible for our quantitative investigations. However, in order to compute the generalized discrepancy as illustrated above, one has to evaluate a series expansion in terms of Legendre polynomials. This summation is very time consuming, in particular, for relatively small s . Therefore, it is not advisable to use this series expansion for the computation of the generalized discrepancy. Fortunately, for certain pseudodifferential operators, the series is representable in terms of elementary functions. One example should be discussed in more detail. Consider the pseudodifferential operator $\mathbf{D} = (-2\Delta^*)^{\frac{1}{2}}(-\Delta^* + \frac{1}{4})^{\frac{1}{4}}$. Its symbol is $\{D_n\}$ with $D_n = \sqrt{(2n+1)n(n+1)}$; its order is $\frac{3}{2}$. Thus, the condition $\mathbf{D}G \in L^2(\Omega)$ is equivalent to $G \in H^{\frac{3}{2}}(\Omega)$; more precisely, $\|\mathbf{D}G\|_{L^2} \leq \sqrt{6}\|G\|_{H^{\frac{3}{2}}}$. It is worth noting that the functions in the Sobolev space $H^{\frac{3}{2}}(\Omega)$ are “slightly smoother” than the continuous functions, and its elements generally are not Lipschitz-continuous. Observing our particular choice the generalized discrepancy is then given by

$$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D}) = \frac{1}{N} \left[\sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \frac{1}{4\pi n(n+1)} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}}.$$

As mentioned above, the series on the right-hand side is expressible in terms of elementary functions

$$(17) \quad D(\{\eta_1, \dots, \eta_N\}; \mathbf{D}) = \frac{1}{2\sqrt{\pi}N} \left[\sum_{i=1}^N \sum_{t=1}^N \left(1 - 2 \ln \left(1 + \sqrt{\frac{1 - \eta_i \cdot \eta_t}{2}} \right) \right) \right]^{\frac{1}{2}}.$$

To keep an appropriate balance between computation and the requirement that the order should be as small as possible, in the following we simply speak of equidistribution on the sphere when $\{\eta_1^N, \dots, \eta_N^N\}$, $N = 1, 2, \dots$, is \mathbf{D} -equidistributed; i.e.,

$$\lim_{N \rightarrow \infty} D(\{\eta_1^N, \dots, \eta_N^N\}; \mathbf{D}) = 0.$$

In connection with Theorem 3.1 we then obtain

$$(18) \quad \left| \frac{1}{4\pi} \int_{\Omega} G(\xi) d\omega(\xi) - \frac{1}{N} \sum_{i=1}^N G(\eta_i) \right| \leq \sqrt{6} D(\{\eta_1, \dots, \eta_N\}; \mathbf{D}) \|G\|_{H^{\frac{3}{2}}},$$

where $D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$ is given by (17) and $G \in H^{\frac{3}{2}}(\Omega)$.

To get an optimal point system on the sphere we have to minimize the expression $D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$ within a set of N points η_1, \dots, η_N on Ω . This is unfortunately a nonlinear optimization problem. It is a challenge for further investigation. Another possibility for construction of pointsets is to require that the sum of some low degree spherical harmonics vanish; that is to say, moments up to a particular order should vanish (see, e.g., [4], [6], [16]).

DEFINITION 3.3 (*m*-design). A pointset $\{\eta_1, \dots, \eta_N\}$ is called an *m*-design if the so-called Weyl sums $\sum_{i=1}^N Y_{n,j}(\eta_i)$ vanish for $n = 1, \dots, m$. To be specific,

$$(19) \quad \sum_{i=1}^N Y_{n,j}(\eta_i) = 0 \quad \text{for } n = 1, 2, \dots, m; j = 1, \dots, 2n+1.$$

Equivalently, a pointset $\{\eta_1, \dots, \eta_N\}$ is an m -design if and only if

$$(20) \quad \frac{1}{4\pi} \int_{\Omega} Y_n(\xi) d\omega(\xi) = \frac{1}{N} \sum_{i=1}^N Y_n(\eta_i)$$

holds for all spherical harmonics Y_n of degree $n \leq m$. It can be shown that a pair of antipodal points, the vertices of a regular tetrahedron, the regular octahedron, and the regular icosahedron give 1-, 2-, 3-, and 5-designs, respectively. In [15] the existence of spherical m -designs is proved but only for sufficiently large N . A construction of m -designs with number of points $N = m^{4.5}$ can be found in [2]. In this paper we only deal with the possibility of an estimate of the generalized discrepancy in the case of an m -design $\{\eta_1, \dots, \eta_N\}$.

LEMMA 3.2. *Let \mathbf{A} be a pseudodifferential operator of order s , $s > 1$ with symbol $\{A_n\}$, $A_n \neq 0$ for $n \geq 1$. If a pointset $\{\eta_1, \dots, \eta_N\}$ is an m -design, then the generalized discrepancy satisfies*

$$D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) \leq \frac{C}{m^{s-1}},$$

where the constant C depends only on s .

Proof. From the definitions of m -design and generalized discrepancy it follows that

$$\begin{aligned} D(\{\eta_1, \dots, \eta_N\}; \mathbf{A}) &= \frac{1}{N} \left[\sum_{i=1}^N \sum_{t=1}^N \sum_{n=1}^{\infty} \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}} \\ &= \frac{1}{N} \left[\sum_{n=m+1}^{\infty} \sum_{i=1}^N \sum_{t=1}^N \frac{2n+1}{4\pi A_n^2} P_n(\eta_i \cdot \eta_t) \right]^{\frac{1}{2}} \\ &\leq \frac{1}{N} \left[\sum_{n=m+1}^{\infty} \sum_{i=1}^N \sum_{t=1}^N \frac{2n+1}{4\pi A_n^2} \right]^{\frac{1}{2}}. \end{aligned}$$

By using the well-known inequality

$$(21) \quad \sum_{n=m+1}^{\infty} \frac{1}{n^s} \leq \frac{C_{z,s}}{m^{s-1}},$$

where the zeta constant is given by $C_{z,s} = \sum_{k=1}^{\infty} \frac{1}{k^s}$, we have the desired estimate. \square

For large values s the m -design gives a good rate of convergence. Suppose that the number of points is $N = m^t$ (for $t \geq 4.5$ we know of the existence of an m -design, but the minimal value of t is unknown); then the rate of convergence amounts to $N^{\frac{s-1}{t}}$. However, for $s = \frac{3}{2}$ and $t = 1$, we obtain a rate of convergence of order $N^{\frac{1}{2}}$. Therefore, this type of m -design does not seem to be well suited.

4. Point systems on the sphere and their discrepancies. Of practical importance is the basic problem of generating a large number of points on the sphere that has a small generalized discrepancy. The geometrical interpretation of a pointset with small generalized discrepancy means that the points in the set are well separated and

TABLE 1
The generalized discrepancy of the simple lattices.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
4	0.0972	1.6817	121	0.0315	0.7211
16	0.0445	1.1222	169	0.0312	0.6762
36	0.0354	0.9320	225	0.0310	0.6415
64	0.0328	0.8218	289	0.0309	0.6138

distributed. A point system is called hierarchical if $\{\eta_1^N, \dots, \eta_N^N\} \subset \{\eta_1^{N+1}, \dots, \eta_{N+1}^{N+1}\}$ for all N . In our approach we distinguish five kinds of point systems on the sphere: lattices in polar coordinates, transformed two-dimensional sequences, rotations on the sphere, triangulations, and the sum of three squares sequence. In this section we briefly describe how these point systems are generated. Then we numerically compute the generalized discrepancies and compare their values. To investigate the order of convergence in a quantitative way, a parameter β determined by

$$(22) \quad D(\{\eta_1, \dots, \eta_N\}; \mathbf{D}) = N^{-\beta}, \quad \text{i.e.,} \quad \beta = -\frac{\log D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})}{\log N},$$

is introduced, where $D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$ is given by (17). A large number of β means that the point system is well structured. The results of the computation exhibit the different orders of convergence for different point systems.

4.1. Conventional polar coordinate lattices. The lattices are generated by taking an equidistant division of the latitude and the longitude. Two examples are considered:

(a) The *simple lattice* $\{(\theta_m, \phi_n); m = 1, \dots, P; n = 1, \dots, Q\}$:

$$\theta_m = m\pi/P, \quad m = 1, 2, \dots, P-1,$$

$$\phi_n = 2n\pi/Q, \quad n = 1, 2, \dots, Q-1.$$

This is the most well known point system in geosciences. Unfortunately, for large numbers P and Q , there is strong concentration of points near the poles. Table 1 gives the computed values of the generalized discrepancy and the factor β for this simple lattice. As expected the point system does not give good results.

(b) To avoid the concentration of points near the poles we keep equidistant laterals

$$\theta_m = m\pi/P, \quad m = 1, 2, \dots, P-1,$$

and divide each lateral circle into

$$n(m) = \text{integer}(2\pi P \sin(m\pi/P))$$

parts; i.e.,

$$\phi_n = 2n\pi/n(m), \quad n = 1, 2, \dots, n(m).$$

Hence, this *improved lattice* does not show strong concentration of points near the poles, since the division of lateral circles depends on the variable θ . The total number of points in the set $\{(\theta_m, \phi_n); m = 1, 2, \dots, P-1, n = 1, 2, \dots, n(m)\}$ amounts to

$$(23) \quad N_P = \sum_{m=1}^{P-1} n(m).$$

Table 2 gives the computed values of the generalized discrepancy and the factor β for the improved lattices. Actually the rate of improvement is slow.

TABLE 2
Generalized discrepancy of the improved lattices.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
6	0.0812	1.4016	234	0.0159	0.7593
20	0.0280	1.194	276	0.0158	0.7382
66	0.0179	0.9600	296	0.0158	0.7294
120	0.0162	0.8610	350	0.0158	0.7079
162	0.0162	0.8099	394	0.0158	0.6943
204	0.0158	0.7797	442	0.0158	0.6811

TABLE 3
Generalized discrepancy of Hammersley systems.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
5	0.0813	1.5590	218	0.0048	0.9919
23	0.0262	1.1612	250	0.0043	0.9874
45	0.0157	1.0908	296	0.0038	0.9779
85	0.0097	1.0427	350	0.0034	0.9712
125	0.0072	1.0218	394	0.0031	0.9671
165	0.0060	1.0035	440	0.0028	0.9637

4.2. Transformed sequences. We again follow the strategy: (i) consider equidistributed pointsets on the rectangle $[-1, 1] \times [0, 2\pi)$; (ii) transform this system via the mapping

$$(t, \phi) \mapsto \xi = (\sqrt{1-t^2} \cos \phi, \sqrt{1-t^2} \sin \phi, t)^T$$

to the unit sphere Ω . As a matter of fact, there are many ways to generate equidistributions in a rectangle (for example, see [8, 9, 10, 13] and many other references).

(a) *Hammersley system*: the p -adic van der Corput sequence is defined by

$$(24) \quad x_n^{(p)} = \frac{a_0}{p} + \dots + \frac{a_r}{p^{r+1}} \quad \text{with} \quad n = a_0 + \dots + a_r p^r,$$

where p is an integer greater than or equal to 2.

Let $t_n = x_n^{(2)}$ be the van der Corput sequence with basis $p = 2$ and $\phi_n = \frac{2n-1}{2N}$. Then the Hammersley system on the sphere is defined by (t_n, ϕ_n) , $n = 1, 2, \dots, N$. The Hammersley system is not hierarchical. A hierarchical point system can be generated by two p -adic van der Corput sequences $(t_n, \phi_n) = (x_n^{(p_1)}, x_n^{(p_2)})$, $n = 1, 2, \dots$, with different prime numbers p_1 and p_2 .

Table 3 gives the computed values of the generalized discrepancy and the factor β for the Hammersley system. The values of β show a significant improvement compared with the former pointsets.

(b) *Uniformly pseudorandom generation*: we use the one-dimensional pseudorandom number generator to determine two sequences (t_j, ϕ_l) , $j, l = 1, 2, \dots$. For example, we choose a classical congruential generator, $x_{n+1} = ax_n \bmod N$ with $a = 31415821$, $N = 10^8$, and $x_0 = 10000$ (see also [18]).

Table 4 gives the computed values of the generalized discrepancy and the factor β for the pseudorandom sequence on the sphere.

4.3. Rotations on the sphere. This so-called *operator sequence* is described in [11]. Let A , B , and C be rotations (orthogonal transformations), respectively, about the X, Y, and Z-axes, each through an angle. Let R_s be the set of nontrivial reduced words in A , B , C , A^{-1} , B^{-1} , C^{-1} of length less than or equal to s (by reduced we

TABLE 4
Generalized discrepancy of pseudorandom sequences.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
22	0.0542	0.9430	222	0.0214	0.7113
62	0.0341	0.8185	262	0.0174	0.7272
102	0.0296	0.7614	302	0.0202	0.6833
142	0.0194	0.7957	342	0.0152	0.7173
202	0.0189	0.7480	402	0.0142	0.7092

TABLE 5
Generalized discrepancy of rotations.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
12	0.0577	1.1478	212	0.0396	0.6026
52	0.0443	0.7887	252	0.0373	0.5948
92	0.0419	0.7015	292	0.0357	0.5872
132	0.0450	0.6353	332	0.0371	0.5676
192	0.0416	0.6048	412	0.0390	0.5387

mean all the obvious cancellations such as AA^{-1} have been carried out); i.e., $R_s = \{A, B, C, A^{-1}, B^{-1}, C^{-1}, AA, AB, AC, AB^{-1}, AC^{-1}, \dots\}$. R_s contains $2N = \frac{3}{2}(5^s - 1)$ elements of rotations. A stereographic projection can be used to relate points in the complex plane \mathbb{C} to points on the sphere. To every point $\xi = (\xi_1, \xi_2, \xi_3)^T$ on the unit sphere, except the north pole $(0, 0, 1)^T$, we associate a complex number

$$(25) \quad z = \frac{\xi_1 + i\xi_2}{1 - \xi_3}.$$

Under this stereographic projection the fractional linear transformations in the complex plane correspond to rotations on the sphere. Taking this into account it is convenient to actually compute with points in \mathbb{C} and fractional linear transformations instead of rotations. In particular, we consider the following fractional linear transformations:

$$A = \frac{1}{\sqrt{5}} \begin{pmatrix} 1+2i & 0 \\ 0 & 1-2i \end{pmatrix}, B = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}, C = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix}.$$

Table 5 gives the computed values of the generalized discrepancy and the factor β with initial complex number i as a starting point for rotations.

4.4. Triangulations. One can generate point systems on the sphere by *triangulation*: the triangulations are initiated with well-known polyhedral corner points of number 4, 8, or 20, which are, respectively, tetrahedron, octahedron, or icosahedron. To refine the triangulation we proceed as follows: connect the midpoints of the sides of each triangle; then project the midpoints on the sphere in a radial direction. This will form four new triangular elements. The points are taken by the center of each new triangular element. Tables 6, 7, 8 give the computed values of the generalized discrepancy and the factor β for triangulations. To our surprise the results are not very convincing for larger pointsets.

4.5. Sum of three squares sequence. This sequence arises in number theory, and a description can be found in [1]. Taking the projection of the integer solutions of the equations $x_1^2 + x_2^2 + x_3^2 = n$, $n \in \mathbb{N}$, on the unit sphere, we are led to sets of type

$$(26) \quad \hat{X}_N = \left\{ \frac{1}{\sqrt{n}}(x_1, x_2, x_3) \mid x_1^2 + x_2^2 + x_3^2 = n; x_1, x_2, x_3 \in \mathbb{Z}, n = 1, 2, \dots, m \right\}.$$

TABLE 6
Generalized discrepancy of tetrahedral triangulation.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
4	0.1115	1.5827
16	0.1038	0.8172
64	0.0723	0.6315
256	0.0712	0.4766
1024	0.0693	0.3851

TABLE 7
Generalized discrepancy of octahedral triangulation.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
8	0.0621	1.3367
32	0.1743	0.5041
128	0.1659	0.3703
512	0.1705	0.2836
2048	0.1753	0.2284

TABLE 8
Generalized discrepancy of icosahedral triangulation.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
20	0.0462	1.0262
80	0.0883	0.5539
320	0.0759	0.4469
1280	0.0792	0.3545

TABLE 9
Generalized discrepancy of the sum of the three squares sequence.

No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β	No. of pts.	$D(\{\eta_1, \dots, \eta_N\}; \mathbf{D})$	β
12	0.1067	0.9006	212	0.0378	0.6116
52	0.0520	0.7484	252	0.0354	0.6041
92	0.0408	0.7077	292	0.0372	0.5797
132	0.0384	0.6678	332	0.0345	0.5800
172	0.0364	0.6325	392	0.0350	0.5613

Removing the redundancy in the set \hat{X}_N we obtain the so-called *sum of three squares sequence* denoted by X_N . This point system is hierarchical, since $X_N \subseteq X_{N+1}$ for all N .

Table 9 gives the computed values of the generalized discrepancy and the factor β for the sum of the three squares sequence. More examples can be found in [3].

4.6. Conclusion. The results of the generalized discrepancy for different types of point systems on the sphere will be plotted below. It is surprising that certain types of transformed sequences yield the best results in our computation. It is also worth mentioning that the triangulations do not take an exceptional role in equidistribution on the sphere (cf. Fig. 1). Furthermore, it should be noted that there exist some well-distributed pointsets with a special number of points on the unit sphere. For example, the soccer ball (the carbon-60 molecule) has the smallest generalized discrepancy ($= 0.0012 \dots$) compared with all our pointsets with about 60 elements.

5. Low discrepancy method. The Monte-Carlo method is very simple; namely, the integral is replaced by its arithmetic mean value over a finite set of points. The

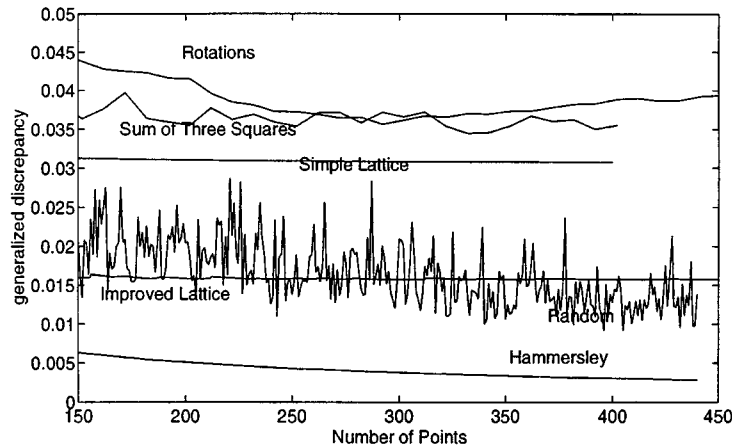


FIG. 1.

TABLE 10
Absolute error of low discrepancy method.

No. of points	Example 1	Example 2	Example 3
100	5.6194e-002	4.3443e-004	2.4112e-002
300	1.4306e-002	4.9351e-005	3.0263e-002
500	5.9281e-003	3.2776e-005	3.5989e-002
700	2.3377e-003	1.4992e-005	2.5217e-003
900	3.4303e-004	1.1899e-005	3.2383e-003
1100	9.2630e-004	5.7437e-006	1.5361e-002
1300	1.8051e-003	4.1731e-006	1.9815e-003
1500	2.4495e-003	3.8074e-006	1.9823e-003

quasi-Monte-Carlo method, sometimes called the low discrepancy method, is understood to be a Monte-Carlo method but based on pointsets forming an equidistribution. The proper justification of the low discrepancy method must not be based on the randomness of the procedure, which is spurious, but on equidistribution of the sets of points at which the values of the integrand are computed. Besides the simplicity, the other advantage of the low discrepancy method is its flexibility in order to guarantee a given accuracy. The transition from N points to $N+1$ points for a hierarchical system needs only one further operation. The drawback of the low discrepancy method is that quite a large number of samplings may be needed, since the convergence tends to be quite slow.

From section 4, empirically we know the factor β . In the following test, the Hammersley point system is used, which turned out in our study to have a good value of β .

Example 1. First we discuss the integration of a discontinuous function, namely the characteristic function given by

$$(27) \quad \chi_h(\xi \cdot \xi_0) = \begin{cases} 1 & \text{if } h \leq \xi \cdot \xi_0 \leq 1, \\ 0 & \text{elsewhere} \end{cases}$$

for fixed $\xi_0 \in \Omega$. The exact value of the integral is easily calculable:

$$(28) \quad \int_{\Omega} \chi_h(\xi \cdot \xi_0) d\omega(\xi) = 2\pi(1 - h).$$

For our tests we choose the parameter $h = \cos(0.1\pi)$ and $\xi_0 = (0, 0, 1)^T$; the exact value of the integral is equal to $0.30752\dots$

Example 2. The second problem deals with the integration of the function (cf. [5])

$$(29) \quad \int_{\Omega} \cos(r\xi_0 \cdot \xi) d\omega(\xi) = 4\pi \frac{\sin(r)}{r}.$$

This function is smooth for small r . For the numerical tests, $r = 1$ and $\xi_0 = (0, 0, 1)^T$ are taken; therefore, we obtain $\int_{\Omega} \cos(r\xi_0 \cdot \xi) d\omega(\xi) = 0.84147\dots$

Example 3. The third problem is concerned with the computation of a highly oscillating integrand. We choose the square of a spherical harmonic with degree $n = 100$ and order $j = 50$. Of course, the integral value of this square of the spherical harmonic is equal to 1.

Table 10 gives an impression of the numerical results.

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