

Quasi–Monte Carlo rules for numerical integration over the unit sphere \mathbb{S}^2

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Received: 28 January 2011 / Revised: 7 November 2011 / Published online: 6 January 2012
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Abstract We study numerical integration on the unit sphere $\mathbb{S}^2 \subseteq \mathbb{R}^3$ using equal weight quadrature rules, where the weights are such that constant functions are integrated exactly. The quadrature points are constructed by lifting a $(0, m, 2)$ -net given in the unit square $[0, 1]^2$ to the sphere \mathbb{S}^2 by means of an area preserving map. A similar approach has previously been suggested by Cui and Freeden [SIAM J Sci Comput 18(2):595–609, 1997]. We prove three results. The first one is that the construction is (almost) optimal with respect to discrepancies based on spherical rectangles. Further we prove that the point set is asymptotically uniformly distributed on \mathbb{S}^2 . And finally, we prove an upper bound on the spherical cap L_2 -discrepancy of order $N^{-1/2}(\log N)^{1/2}$ (where N denotes the number of points). This improves upon the bound on the spherical cap L_2 -discrepancy of the construction by Lubotzky, Phillips and Sarnak [Commun Pure Appl Math 39(S, suppl):S149–S186, 1986] by a factor of $\sqrt{\log N}$. Numerical results suggest that the $(0, m, 2)$ -nets lifted to the sphere \mathbb{S}^2 have spherical cap L_2 -discrepancy converging with the optimal order of $N^{-3/4}$.

Mathematics Subject Classification (2000) 65D30 · 65D32

J.S. Brauchart is supported by an APART-Fellowship of the Austrian Academy of Sciences. J. Dick is supported by an Australian Research Council Queen Elizabeth 2 Fellowship.

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1 Introduction

We consider the unit sphere $\mathbb{S}^2 = \{z = (z_1, z_2, z_3) \in \mathbb{R}^3 : \|z\| = \sqrt{z_1^2 + z_2^2 + z_3^2} = 1\}$. Let $f : \mathbb{S}^2 \rightarrow \mathbb{R}$ be integrable. Then we estimate the integral $\int_{\mathbb{S}^2} f \, d\sigma_2$, where σ_2 is the normalized Lebesgue surface area measure (that is $\int_{\mathbb{S}^2} d\sigma_2 = 1$), by a Quasi-Monte Carlo type rule

$$Q_N(f) = \frac{1}{N} \sum_{k=0}^{N-1} f(z_k),$$

where $Z_N = \{z_0, \dots, z_{N-1}\} \subseteq \mathbb{S}^2$ are the quadrature points on the sphere. Since the surface area measure is normalized to 1, it follows that we have $Q_N(f) = \int_{\mathbb{S}^2} f \, d\sigma_2$ for every constant function f . In the following we review known results to put the result of this paper into context. Although some results are known for spheres \mathbb{S}^d of dimension $d \geq 2$, we only state them for the sphere \mathbb{S}^2 since this paper only deals with the 2-sphere.

Using Stolarsky's invariance principle [40] (also see [10] and [11]), it follows that the worst-case error for numerical integration in a certain reproducing kernel Hilbert space is given by the spherical cap L_2 -discrepancy of the quadrature points. To obtain quadrature points we use a transformation from $[0, 1]^2$ to \mathbb{S}^2 which preserves area. Specifically, we use the transformation $\Phi : [0, 1]^2 \rightarrow \mathbb{S}^2$ with

$$\Phi(y_1, y_2) = \left(2 \cos(2\pi y_1) \sqrt{y_2 - y_2^2}, 2 \sin(2\pi y_1) \sqrt{y_2 - y_2^2}, 1 - 2y_2 \right).$$

The function Φ maps axis-parallel rectangles in the unit square to zonal spherical rectangles of equal area. It is natural then that the discrepancy on the sphere with respect to spherical rectangles is the same as the discrepancy with respect to rectangles in $[0, 1]^2$. Since point sets Z_N for which a discrepancy based on K -regular test sets (K fixed, see Sjögren [37]) converges to zero as $N \rightarrow \infty$ are uniformly distributed over the sphere, we show that the digital nets lifted to the sphere via Φ are also uniformly distributed.

Furthermore, we study the spherical cap L_2 -discrepancy of point sets obtained in this way. We prove that the order of convergence for $(0, m, 2)$ -nets lifted to the sphere via Φ is $\mathcal{O}(N^{-1/2}(\log N)^{1/2})$. This improves upon the bound on the spherical cap L_2 -discrepancy in [26] of $\mathcal{O}(N^{-1/2} \log N)$ by a factor of $\sqrt{\log N}$. On the other hand, the optimal order of convergence is $\mathcal{O}(N^{-3/4})$. But numerical experiments do suggest that the $(0, m, 2)$ -nets lifted to the sphere via Φ achieve optimal convergence rate. We conjecture that this order of convergence is the correct one.

Due to the difficulties of having a satisfactory notion of 'bounded variation' on \mathbb{S}^2 there is no Koksma–Hlawka inequality on \mathbb{S}^2 per se. However, the concept of *uniform distribution of a sequence of N -point configurations with respect to every function in a function space*, say Sobolev spaces over \mathbb{S}^2 , can be used as quality criterion. For example, Cui and Freeden [13] introduced the concept of a generalized discrepancy on \mathbb{S}^2 which involves pseudodifferential operators. Using the operator

$\mathbf{D} = (-2\Delta^*)^{1/2}(-\Delta^* + 1/4)^{1/4}$ (Δ^* is the Beltrami operator on \mathbb{S}^2) of order $3/2$ they arrived at

$$\left| \frac{1}{N} \sum_{k=1}^N f(\mathbf{x}_k) - \int f \, d\sigma_2 \right| \leq \sqrt{6} D(\{\mathbf{x}_1, \dots, \mathbf{x}_N\}; \mathbf{D}) \|f\|_{\mathcal{H}^{3/2}},$$

where f is from the Sobolev space $\mathcal{H}^{3/2}(\mathbb{S}^2)$. In this notion, a sequence $\{Z_N\}$ of N -point configurations is called **D**-equidistributed in $\mathcal{H}^{3/2}(\mathbb{S}^2)$ if $\lim_{N \rightarrow \infty} D(\{z_1, \dots, z_N\}; \mathbf{D}) = 0$. The generalized discrepancy associated with **D** can be easily computed by way of

$$4\pi [D(\{z_1, \dots, z_N\}; \mathbf{D})]^2 = 1 - \frac{1}{N^2} \sum_{k, \ell=1}^N \log(1 + \|z_\ell - z_k\|/2)^2. \quad (1)$$

Sloan and Womersley [38] showed that $[D(\{z_1, \dots, z_N\}; \mathbf{D})]^2$ has a natural interpretation as the worst-case error for the equally weighted quadrature rule Q_N associated with the points z_1, \dots, z_N for functions f from the unit ball in $\mathcal{H}^{3/2}(\mathbb{S}^2)$ provided with the reproducing kernel $K(\mathbf{y}, \mathbf{z}) = 2[1 - \log(1 + \|\mathbf{y} - \mathbf{z}\|/2)]$. In [11] this approach is followed further, yielding an even simpler notion of discrepancy (see Sect. 3), namely

$$[D(\{z_1, \dots, z_N\})]^2 = \frac{4}{3} - \frac{1}{N^2} \sum_{k, \ell=1}^N \|z_\ell - z_k\| \quad (2)$$

also used in the setting of the Sobolev space $\mathcal{H}^{3/2}(\mathbb{S}^2)$ now provided with the reproducing kernel $K(\mathbf{y}, \mathbf{z}) = (8/3) - \|\mathbf{y} - \mathbf{z}\|$. Low-discrepancy configurations in the above contexts can be found by maximizing the respective double sums in (1) and (2). This leads into the realm of the discrete (minimum) energy problem on the sphere where points are thought to interact according to a Riesz s -potential $1/r^s$ ($s > 0$) or logarithmic potential $\log(1/r)$ ($s = 0$) and r is the Euclidean distance in the ambient space. It is known that the minimizer Z_N ($N \geq 2$) of the associated s -energy functionals form a sequence which is asymptotically uniformly distributed for each fixed $s \geq 0$. We refer the interested reader to [3, 5–7, 9, 12, 20, 21, 42–44]. We remark that Sun and Chen [41] employ ‘spherical basis functions’ (as a counter part to radial basis function on spheres) to investigate uniform distribution on spheres. They also show that the minimizers of the functionals induced by a spherical basis function are asymptotically uniformly distributed.

Let $C(\mathbf{z}, t) := \{\mathbf{y} \in \mathbb{S}^2 : \langle \mathbf{y}, \mathbf{z} \rangle \leq t\}$ be a spherical cap and let $\mathcal{C} := \{C(\mathbf{z}, t) : \mathbf{z} \in \mathbb{S}^2, -1 \leq t \leq 1\}$ denote the set of all spherical caps. In [40], Stolarsky established a beautiful invariance principle on the 2-sphere (and higher-dimensional spheres),

$$\frac{1}{N^2} \sum_{k, \ell=1}^N \|z_\ell - z_k\| + 4[D_2(Z_N; \mathbb{S}^2, \mathcal{C})]^2 = \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \|\mathbf{y} - \mathbf{z}\| \, d\sigma_2(\mathbf{y}) \, d\sigma_2(\mathbf{z}), \quad (3)$$

connecting the sum of distances, the L_2 -discrepancy (with respect to spherical caps $C(\mathbf{z}, t)$),

$$D_2(Z_N; \mathbb{S}^2, C) := \left[\int_{-1}^1 \int_{\mathbb{S}^2} \left| \frac{|Z_N \cap C(\mathbf{z}, t)|}{N} - \sigma_2(C(\mathbf{z}, t)) \right|^2 d\sigma_2(\mathbf{z}) dt \right]^{1/2},$$

and the distance integral. We observe that, on \mathbb{S}^2 , the discrepancy in (2) is essentially (up to a factor 2) the L_2 -discrepancy. Originally, Stolarsky used his invariance principle and sharp result for discrepancy estimates by Schmidt [36] to establish bounds for the sum of distances. Beck [4] then improved Stolarsky's lower bound, finally arriving at

$$c N^{-3/2} \leq \int \int \|\mathbf{x} - \mathbf{y}\| d\sigma_2(\mathbf{x}) d\sigma_2(\mathbf{y}) - \frac{1}{N^2} \sum_{k, \ell=1}^N \|\mathbf{z}_\ell - \mathbf{z}_k\| \leq C N^{-3/2} \quad (4)$$

for some universal positive constants c and C independent of N . Consequently, relations (4) yield lower and upper bound for the L_2 -discrepancy by means of the invariance principle which are sharp with respect to order of N :

$$c' N^{-3/4} \leq D_2(Z_N^*; \mathbb{S}^2, C) \leq C' N^{-3/4}$$

for a sequence of optimal L_2 -discrepancy N -point configurations Z_N^* on \mathbb{S}^2 . Observe, that optimal L_2 -discrepancy and optimal spherical cap discrepancy configurations satisfy estimates with the same order $N^{-3/4}$ (apart from a possible $\sqrt{\log N}$ term), see [4].

1.1 Quasi-Monte Carlo rules in the unit square

Quasi-Monte Carlo algorithms $\widehat{I}(f) = \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n)$ are used to approximate integrals $I(f) = \int_{[0,1]^2} f(\mathbf{x}) d\mathbf{x}$. The crux of the method is to choose the quadrature points $\mathbf{x}_0, \dots, \mathbf{x}_{N-1}$ as uniformly distributed as possible. The difference to Monte Carlo is the method by which the sample points $\mathbf{x}_0, \dots, \mathbf{x}_{N-1} \in [0, 1]^2$ are chosen. The aim of QMC is to choose those points such that the integration error

$$\left| \int_{[0,1]^2} f(\mathbf{x}) d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n) \right|$$

achieves the (almost) optimal rate of convergence as $N \rightarrow \infty$ for certain classes of functions $f : [0, 1]^2 \rightarrow \mathbb{R}$. For instance, for the family of functions f with bounded variation in the sense of Hardy and Krause (for which we write $\|f\|_{\text{HK}} < \infty$) it is

known that the best rate of convergence for the worst case error is

$$e = \sup_{f, \|f\|_{\text{HK}} < \infty} \left| \int_{[0,1]^2} f(\mathbf{x}) \, d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n) \right| \asymp N^{-1+\varepsilon} \quad \text{for all } \varepsilon > 0.$$

More precisely, there are constants $c, C > 0$ such that

$$cN^{-1} \sqrt{\log N} \leq e \leq CN^{-1} \sqrt{\log N},$$

see [15].

There is an explicit construction of the sample points $\mathbf{x}_0, \dots, \mathbf{x}_{N-1}$ for which the optimal rate of convergence is achieved. One criterion for how uniformly a set of points $P_N = \{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\}$ is distributed in the unit square is the star discrepancy

$$D^*(P_N; [0, 1]^2, \mathcal{R}^*) = \sup_{\mathbf{y} \in [0, 1]^2} |\delta_{P_N}(\mathbf{y})|, \quad \delta_{P_N}(\mathbf{y}) = \frac{1}{N} \sum_{n=0}^{N-1} 1_{\mathbf{x}_i \in [\mathbf{0}, \mathbf{y})} - \text{Area}([\mathbf{0}, \mathbf{y})),$$

where $[\mathbf{0}, \mathbf{y}) = \prod_{i=1}^s [0, y_i)$ with $\mathbf{y} = (y_1, y_2) \in [0, 1]^2$, $\mathcal{R}^* = \{[\mathbf{0}, \mathbf{y}) : \mathbf{y} \in [0, 1]^2\}$, $\text{Area}([\mathbf{0}, \mathbf{y})) = y_1 y_2$ is the area of $[\mathbf{0}, \mathbf{y})$ and

$$1_{\mathbf{x}_i \in [\mathbf{0}, \mathbf{y})} = \begin{cases} 1 & \text{if } \mathbf{x}_i \in [\mathbf{0}, \mathbf{y}), \\ 0 & \text{otherwise.} \end{cases}$$

The quantity $\delta_{P_N}(\mathbf{y})$ is called the local discrepancy (of P_N).

The connection between this criterion and the integration error is given by the Koksma–Hlawka inequality

$$\left| \int_{[0,1]^2} f(\mathbf{x}) \, d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n) \right| \leq D^*(P_N; [0, 1]^2, \mathcal{R}^*) \|f\|_{\text{HK}}.$$

Informally, a sequence of points $\mathbf{x}_0, \mathbf{x}_1, \dots \in [0, 1)^s$ is called a low-discrepancy sequence, if

$$D^*(\{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\}; [0, 1]^2, \mathcal{R}^*) = \mathcal{O}(N^{-1}(\log N)^2) \quad \text{as } N \rightarrow \infty.$$

Notice that for such a point sequence, the Koksma–Hlawka inequality implies the optimal rate of convergence of the integration error (apart from the power of the $\log N$ factor), since for a given integrand f the variation $\|f\|_{\text{HK}}$ does not depend on P_N and N at all.

The concept of digital nets introduced by Niederreiter [30] provides the to date most efficient method to explicitly construct points sets $P_N = \{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\} \in [0, 1)^2$

with small discrepancy, that is

$$D^*(P_N; [0, 1]^2, \mathcal{R}^*) \leq CN^{-1} \log N.$$

They are introduced in the next section.

1.2 Nets and sequences in the unit square

In this section we give a brief overview of (digital) $(0, m, 2)$ -nets and (digital) $(0, 2)$ -sequences. For a comprehensive introduction see [15].

The aim is to construct a point set $P_N = \{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\}$ such that the star discrepancy satisfies $D^*(P_N; [0, 1]^2, \mathcal{R}^*) \leq CN^{-1} \log N$. To do so, we discretize the problem by choosing the point set P_N such that the local discrepancy $\delta_{P_N}(\mathbf{y}) = 0$ for certain $\mathbf{y} \in [0, 1]^2$ (those \mathbf{y} in turn are chosen such that the star discrepancy of P_N is small, as we explain below).

It turns out that, when one chooses a base $b \geq 2$ and $N = b^m$, then for every natural number m there exist point sets $P_{b^m} = \{\mathbf{x}_0, \dots, \mathbf{x}_{b^m-1}\}$ such that $\delta_{P_{b^m}}(\mathbf{y}) = 0$ for all $\mathbf{y} = (y_1, y_2)$ of the form

$$y_i = a_i / b^{d_i} \quad \text{for } i = 1, 2,$$

where $0 < a_i \leq b^{d_i}$ is an integer and $d_1 + d_2 \leq m$ with $d_1, d_2 \geq 0$. A point set P_N which satisfies this property is called a $(0, m, 2)$ -net in base b . An equivalent description of $(0, m, 2)$ -nets in base b is given in the following definition.

Definition 1 Let $b \geq 2$ and $m \geq 1$ be integers. A point set $P_{b^m} \subseteq [0, 1)^2$ consisting of b^m points is called a $(0, m, 2)$ -net in base b , if for all nonnegative integers d_1, d_2 with $d_1 + d_2 = m$, the elementary interval

$$\prod_{i=1}^2 \left[\frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right)$$

contains exactly 1 point of P_{b^m} for all integers $0 \leq a_i < b^{d_i}$.

It is also possible to construct nested $(0, m, 2)$ -nets, thereby obtaining an infinite sequence of points.

Definition 2 Let $b \geq 2$ be an integer. A sequence $\mathbf{x}_0, \mathbf{x}_1, \dots \in [0, 1)^2$ is called a $(0, 2)$ -sequence in base b , if for all $m > 0$ and for all $k \geq 0$, the point set $\mathbf{x}_{kb^m}, \mathbf{x}_{kb^m+1}, \dots, \mathbf{x}_{(k+1)b^m-1}$ is a $(0, m, 2)$ -net in base b .

It can be shown that a $(0, m, 2)$ -net in base b satisfies

$$D^*(P_N; [0, 1]^2, \mathcal{R}^*) \leq C_b \frac{m}{b^{m-1}},$$

and the first N points $\mathbf{x}_0, \dots, \mathbf{x}_{N-1}$ of a $(0, 2)$ -sequence in base b satisfy

$$D^*({\mathbf{x}}_0, \dots, {\mathbf{x}}_{N-1}; [0, 1]^2, \mathcal{R}^*) \leq C_b \frac{(\log N)^2}{N} \quad \text{for all } N \geq 1,$$

where $C_b > 0$ depends on b but not on m and N . See [15, 31] for details.

Explicit constructions of $(0, m, 2)$ -nets and $(0, 2)$ -sequences can be obtained using the digital construction scheme. Such point sets are then called digital nets [or digital $(0, m, 2)$ -nets if the point set is a $(0, m, 2)$ -net] or digital sequences [or digital $(0, 2)$ -sequence if the sequence is a $(0, 2)$ -sequence].

To describe the digital construction scheme, let b be a prime number and let \mathbb{Z}_b be the finite field of order b (a prime power and the finite field \mathbb{F}_b could be used as well). Let $C_1, C_2 \in \mathbb{Z}_b^{m \times m}$ be 2 matrices of size $m \times m$ with elements in \mathbb{Z}_b . The i th coordinate $x_{n,i}$ of the n th point $\mathbf{x}_n = (x_{n,1}, x_{n,2})$ of the digital net is obtained in the following way. For $0 \leq n < b^m$ let $n = n_0 + n_1b + \dots + n_{m-1}b^{m-1}$ be the base b representation of n . Let $\vec{n} = (n_0, \dots, n_{m-1})^\top \in \mathbb{Z}_b^m$ denote the vector of digits of n . Then let

$$\vec{y}_{n,i} = C_i \vec{n}.$$

For $\vec{y}_{n,i} = (y_{n,i,1}, \dots, y_{n,i,m})^\top \in \mathbb{Z}_b^m$ we set

$$x_{n,i} = \frac{y_{n,i,1}}{b} + \dots + \frac{y_{n,i,m}}{b^m}.$$

To construct digital sequences, the generating matrices C_1, C_2 are of size $\infty \times \infty$.

The search for $(0, m, 2)$ -nets and $(0, 2)$ -sequences has now been reduced to finding suitable matrices C_1, C_2 . Explicit constructions of such matrices are available and where introduced (in chronological order) by Sobol [39], Faure [18], Niederreiter [30], Niederreiter and Xing [32, 33, 45], as well as others. For instance, to obtain a digital $(0, m, 2)$ -net over \mathbb{Z}_2 one can choose

$$C_1 = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \ddots & & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & & \ddots & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} \quad \text{and} \quad C_2 = \begin{pmatrix} \binom{0}{0} & \binom{1}{0} & \dots & \dots & \binom{m-1}{0} \\ 0 & \binom{1}{1} & \dots & \dots & \binom{m-1}{1} \\ \vdots & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & \binom{m-2}{m-2} & \binom{m-1}{m-2} \\ 0 & \dots & \dots & 0 & \binom{m-1}{m-1} \end{pmatrix},$$

where the binomial coefficients are taken modulo 2. Notice that the matrices C_1, C_2 can be extended to $\infty \times \infty$ matrices yielding generating matrices for a digital $(0, 2)$ -sequence over \mathbb{Z}_2 . This example was first provided by Sobol' in [39].

2 Spherical rectangle discrepancy of point sets on the unit sphere \mathbb{S}^2

We introduce a transformation to lift $(0, m, 2)$ -nets to the sphere \mathbb{S}^2 . To do so, we represent each point on the sphere \mathbb{S}^2 by using scaled spherical coordinates. We define $T : [0, 1) \times [0, 1] \mapsto \mathbb{S}^2$ by

$$T(\theta, \phi) = (\cos(2\pi\theta) \sin(\pi\phi), \sin(2\pi\theta) \sin(\pi\phi), \cos(\pi\phi)).$$

Let $0 \leq \theta_1 \leq \theta \leq \theta_2 \leq 1$ and $0 \leq \phi_1 \leq \phi_2 \leq 1$. The part of the sphere

$$\Omega_{\theta_1, \theta_2, \phi_1, \phi_2} = \{T(\theta, \phi) \in \mathbb{S}^2 : \theta_1 \leq \theta < \theta_2, \phi_1 \leq \phi < \phi_2\}$$

has area

$$\text{Area}(\Omega_{\theta_1, \theta_2, \phi_1, \phi_2}) = 2\pi(\theta_2 - \theta_1)[\cos(\pi\phi_1) - \cos(\pi\phi_2)].$$

Let

$$\Gamma_{\theta_1, \theta_2, \phi_1, \phi_2} := \frac{\text{Area}(\Omega_{\theta_1, \theta_2, \phi_1, \phi_2})}{\text{Area}(\mathbb{S}^2)} = (\theta_2 - \theta_1) \frac{\cos(\pi\phi_1) - \cos(\pi\phi_2)}{2},$$

be the area of $\Omega_{\theta_1, \theta_2, \phi_1, \phi_2}$ normalized with respect to the surface area of the unit sphere. Therefore we have $\Gamma_{0,1,0,1} = 1$. We can now define a discrepancy measure of point sets on the sphere with respect to sets $\Omega_{\theta_1, \theta_2, \phi_1, \phi_2}$.

Definition 3 Let $Z_N = \{z_0, \dots, z_{N-1}\} \subseteq \mathbb{S}^2$. Then the extreme spherical rectangle discrepancy of Z_N on \mathbb{S}^2 with respect to $\Omega = \{\Omega_{\theta_1, \theta_2, \phi_1, \phi_2} : 0 \leq \theta_1 < \theta_2 \leq 1, 0 \leq \phi_1 < \phi_2 \leq 1\}$ is defined by

$$D_N(Z_N; \mathbb{S}^2, \Omega) = \sup_{\substack{0 \leq \theta_1 < \theta_2 \leq 1 \\ 0 \leq \phi_1 < \phi_2 \leq 1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{\theta_1, \theta_2, \phi_1, \phi_2}} - \Gamma_{\theta_1, \theta_2, \phi_1, \phi_2} \right|,$$

where

$$1_{z_n \in \Omega_{\theta_1, \theta_2, \phi_1, \phi_2}} = \begin{cases} 1 & \text{if } z_n \in \Omega_{\theta_1, \theta_2, \phi_1, \phi_2} \\ 0 & \text{otherwise.} \end{cases}$$

The spherical rectangle star-discrepancy of Z_N on \mathbb{S}^2 with respect to $\Omega^* = \{\Omega_{0, \theta, 0, \phi} : 0 \leq \theta \leq 1, 0 \leq \phi \leq 1\}$ is defined by

$$D_N^*(Z_N; \mathbb{S}^2, \Omega^*) = \sup_{\substack{0 \leq \theta \leq 1 \\ 0 \leq \phi \leq 1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{0, \theta, 0, \phi}} - \Gamma_{0, \theta, 0, \phi} \right|.$$

The expression $\frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{\theta_1, \theta_2, \phi_1, \phi_2}}$ denotes the proportion of points of Z_N in $\Omega_{\theta_1, \theta_2, \phi_1, \phi_2}$. Note that the set $\Omega_{\theta_1, \theta_2, \phi_1, \phi_2}$ always includes the North Pole $(0, 0, 1)$ and never the South Pole $(0, 0, -1)$.

Further, the discrepancy measure includes the discrepancy of spherical caps centered at the North Pole $(0, 0, 1)$ and South Pole $(0, 0, -1)$. The spherical cap at the North Pole is obtained by using $\Omega_{0,1,0,\phi}$. Let $\phi > 0$ be small. Then $\frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{0,1,0,\phi}}$ is the proportion of points in the spherical cap $\Omega_{0,1,0,\phi}$ and $4\pi \Gamma_{0,1,0,\phi}$ is the area of the spherical cap. Hence

$$\left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{0,1,0,\phi}} - \Gamma_{0,1,0,\phi} \right|$$

measures the discrepancy at the North Pole. The South Pole is included in the following way. Let $\phi < 1$ be close to 1. Then $\mathbb{S}^2 \setminus \Omega_{0,1,0,\phi}$ is the spherical cap centered at the South Pole. Then

$$\frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \mathbb{S}^2 \setminus \Omega_{0,1,0,\phi}} = 1 - \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{0,1,0,\phi}}$$

is the proportion of points in the spherical cap centered at the South Pole. Further, $4\pi(1 - \Gamma_{0,1,0,\phi})$ is the area of the spherical cap $\mathbb{S}^2 \setminus \Omega_{0,1,0,\phi}$. Hence

$$\left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \Omega_{0,1,0,\phi}} - \Gamma_{0,1,0,\phi} \right| = \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{z_n \in \mathbb{S}^2 \setminus \Omega_{0,1,0,\phi}} - \frac{\text{Area}(\mathbb{S}^2 \setminus \Omega_{0,1,0,\phi})}{\text{Area}(\mathbb{S}^2)} \right|$$

measures the discrepancy at the South Pole.

In the following we construct point sets $Z_N = \{z_0, \dots, z_{N-1}\}$ on the sphere \mathbb{S}^2 such that $D_N(Z_N; \mathbb{S}^2, \Omega)$ is small. This can be done by relating the spherical rectangle discrepancy to an analogous discrepancy on $[0, 1]^2$.

Definition 4 Let $P_N = \{x_0, \dots, x_{N-1}\} \subseteq [0, 1]^2$. Then the extreme discrepancy of P_N on $[0, 1]^2$ with respect to $\mathcal{R} = \{[a_1, a_2) \times [c_1, c_2) : 0 \leq a_1 < a_2 \leq 1, 0 \leq c_1 < c_2 \leq 1\}$ is defined by

$$D(P_N; [0, 1]^2, \mathcal{R}) = \sup_{\substack{0 \leq a_1 < a_2 \leq 1 \\ 0 \leq c_1 < c_2 \leq 1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{x_n \in [a_1, a_2) \times [c_1, c_2)} - (a_2 - a_1)(c_2 - c_1) \right|,$$

where

$$1_{x_n \in [a_1, a_2) \times [c_1, c_2)} = \begin{cases} 1 & \text{if } x_n \in [a_1, a_2) \times [c_1, c_2), \\ 0 & \text{otherwise.} \end{cases}$$

The star-discrepancy of P_N on $[0, 1)^2$ with respect to $\mathcal{R}^* = \{[0, a) \times [0, c) : 0 \leq a \leq 1, 0 \leq c \leq 1\}$ is defined by

$$D^*(P_N; [0, 1)^2, \mathcal{R}^*) = \sup_{\substack{0 \leq a \leq 1 \\ 0 \leq c \leq 1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} 1_{\mathbf{x}_n \in [0, a) \times [0, c)} - ac \right|.$$

Let P_N be an arbitrary point set in $[0, 1)^2$. It is known, see for instance [15, Chapter 3], that

$$D^*(P_N; [0, 1)^2, \mathcal{R}^*) \leq D_N(P_N; [0, 1)^2, \mathcal{R}) \leq 4D^*(P_N; [0, 1)^2, \mathcal{R}^*).$$

The following lemma establishes a connection between the discrepancies on $[0, 1)^2$ and \mathbb{S}^2 defined above.

Lemma 1 Let $P_N = \{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\} \in (0, 1)^2$ and $\mathbf{x}_n = (x_{n,1}, x_{n,2})$ for $0 \leq n < N$. Let

$$\mathbf{z}_n = T\left(x_{n,1}, \frac{\arccos(1 - 2x_{n,2})}{\pi}\right) \text{ for } 0 \leq n < N$$

and $Z_N = \{\mathbf{z}_0, \dots, \mathbf{z}_{N-1}\}$. Then $\mathbf{z}_n \in \mathbb{S}^2$ for $0 \leq n < N$ and

$$D_N(Z_N; \mathbb{S}^2, \Omega) = D_N(P_N; [0, 1)^2, \mathcal{R})$$

and

$$D_N^*(Z_N; \mathbb{S}^2, \Omega^*) = D_N(P_N; [0, 1)^2, \mathcal{R}^*).$$

Proof It is trivial to check that $\|\mathbf{z}_n\| = 1$ for all n . To show the second part, we set $\theta_1 = a_1, \theta_2 = a_2, \phi_1 = [\arccos(1 - 2c_1)]/\pi$ and $\phi_2 = [\arccos(1 - 2c_2)]/\pi$. Then we have

$$\Gamma_{\theta_1, \theta_2, \phi_1, \phi_2} = (a_2 - a_1) \frac{1 - 2c_1 - (1 - 2c_2)}{2} = (a_2 - a_1)(c_2 - c_1). \quad (5)$$

Note that the points $(0, 0, 1)$ and $(0, 0, -1)$ are excluded from the set Z_N since we assume that $P_N \subseteq (0, 1)^2$. The mapping from P_N to Z_N is therefore bijective. Therefore we have

$$1_{\mathbf{z}_n \in \Omega_{\theta_1, \theta_2, \phi_1, \phi_2}} = 1_{(y_{n,1}, (\arccos(1 - 2y_{n,2}))/\pi) \in [\theta_1, \theta_2) \times [\phi_1, \phi_2)} = 1_{(y_{n,1}, y_{n,2}) \in [a_1, a_2) \times [c_1, c_2)}.$$

Thus the remaining results follow from Definitions 3 and 4. \square

Remark 1 Note that $\sin(\arccos(1 - 2x)) = \sqrt{x - x^2}$, whence $\mathbf{z}_n = (z_{n,1}, z_{n,2}, z_{n,3})$ where

$$z_{n,1} = 2 \cos(2\pi x_{n,1}) \sqrt{x_{n,2} - x_{n,2}^2},$$

$$\begin{aligned} z_{n,2} &= 2 \sin(2\pi x_{n,1}) \sqrt{x_{n,2} - x_{n,2}^2}, \\ z_{n,3} &= 1 - 2x_{n,2} \end{aligned}$$

for $0 \leq n < N$. To shorten the notation we define

$$\begin{aligned} \Phi(x_1, x_2) &= T\left(x_1, \frac{\arccos(1 - 2x_2)}{\pi}\right) \\ &= \left(2 \cos(2\pi x_1) \sqrt{x_2 - x_2^2}, 2 \sin(2\pi x_1) \sqrt{x_2 - x_2^2}, 1 - 2x_2\right) \end{aligned}$$

for $(x_1, x_2) \in [0, 1]^2$. Hence, $z_n = \Phi(\mathbf{x}_n)$ for $0 \leq n < b^m$.

Further, for $J \subseteq [0, 1]^2$ we set

$$\Phi(J) = \{\Phi(\mathbf{x}) \in \mathbb{S}^2 : \mathbf{x} \in J\}.$$

2.1 Digital nets on the sphere

The previous lemma can now be used to obtain a bound on the spherical rectangle discrepancy of $(0, m, 2)$ -nets lifted to the sphere via the transformation Φ , which we state in the following result.

Theorem 1 *Let $P_N = \{\mathbf{x}_0, \dots, \mathbf{x}_{b^m-1}\} \subseteq (0, 1)^2$ be a $(0, m, 2)$ -net in base b . Let $\mathbf{x}_n = (x_{n,1}, x_{n,2})$ for $0 \leq n < b^m$. Let $z_n = \Phi(\mathbf{x}_n)$ for $0 \leq n < b^m$ and $Z_N = \{z_0, \dots, z_{b^m-1}\}$. Then*

$$D_{b^m}(Z_N; \mathbb{S}^2, \Omega) \leq \frac{b^2}{b+1} \frac{m}{b^m} + \frac{1}{b^m} \left(9 + \frac{1}{b}\right) + \frac{1}{b^{2m}} \left(2b - 1 - \frac{4b+3}{(b+1)^2}\right)$$

and

$$D_{b^m}^*(Z_N; \mathbb{S}^2, \Omega^*) \leq \frac{b^2}{b+1} \frac{m}{4b^m} + \frac{1}{b^m} \left(\frac{9}{4} + \frac{1}{b}\right) + \frac{1}{b^{2m}} \left(\frac{b}{2} - \frac{1}{4} - \frac{4b+3}{4(b+1)^2}\right).$$

Proof The result follows from Lemma 1 and [14, Theorem 1 and Remark 2]. \square

Lemma 1 and the result of Roth [35] imply that

$$D_N(Z_N; \mathbb{S}^2, \Omega) \geq D_N^*(Z_N; \mathbb{S}^2, \Omega^*) \geq \frac{\lfloor \log_2 N \rfloor + 3}{2^8 N}$$

for all point sets $Z_N = \{z_0, \dots, z_{N-1}\} \subseteq \mathbb{S}^2$ (where \log_2 denotes the logarithm in base 2). Thus the construction of Theorem 1 is optimal with respect to the discrepancy defined in Definition 3.

Theorem 1 is not surprising since the transformation Φ is area preserving for all rectangles, which follows from (5).

2.2 Uniform distribution on the sphere

A sequence of N -point systems $\{Z_N\}_{N \geq 2}$ on the unit sphere \mathbb{S}^2 in \mathbb{R}^3 is said to be *asymptotically uniformly distributed on \mathbb{S}^2* if the exact integral $I(f) = \int_{\mathbb{S}^2} f \, d\sigma_2$ of any continuous function f on \mathbb{S}^2 integrated with respect to the normalized surface area measure σ_2 on \mathbb{S}^2 can be approximated arbitrarily close (as N becomes large) by means of the equally weighted quadrature rules Q_N having these Z_N as node sets; that is

$$\lim_{N \rightarrow \infty} Q_N(f) = I(f) \quad \text{for every } f \in C(\mathbb{S}^2).$$

This limit relation also states that the weak-* limit (which is defined in such a way) of the discrete measure placing a point mass $1/N$ at every point in Z_N is given by the natural measure on \mathbb{S}^2 . In other words, the limit distribution (as $N \rightarrow \infty$) of the N -point configurations Z_N is given by σ_2 . Let $|Z_N|$ denote the cardinality of the (finite) set Z_N . Therefore, an equivalent characterization is that

$$\lim_{N \rightarrow \infty} |Z_N \cap A|/N = \sigma_2(A)$$

for every σ_2 -measurable set $A \subseteq \mathbb{S}^2$ (whose boundary has 2-dimensional Hausdorff measure 0). Informally speaking, any such set A gets a fair share of points as N becomes large. In fact, it is sufficient to consider spherical caps on \mathbb{S}^2 . Let $\mathcal{C} = \{C(\mathbf{z}, t) : \mathbf{z} \in \mathbb{S}^2, -1 \leq t \leq 1\}$ denote the set of all spherical caps. Thus, a natural measure to quantify 'equidistribution' of N -point systems on \mathbb{S}^2 is the *spherical cap discrepancy*

$$D(Z_N; \mathbb{S}^2, \mathcal{C}) := \sup_{C \in \mathcal{C}} \left| \frac{|Z_N \cap C|}{N} - \sigma_2(C) \right|,$$

where the supremum is extended over all spherical caps. It is well-known that the sequence $\{Z_N\}_{N \geq 2}$ is asymptotically uniformly distributed on \mathbb{S}^2 if and only if $D(Z_N; \mathbb{S}^2, \mathcal{C}) \rightarrow 0$ as $N \rightarrow \infty$. One can show that the following assertions are equivalent (cf., for example, [9]):

1. The sequence $\{Z_N\}_{N \geq 2}$ is asymptotically uniformly distributed on \mathbb{S}^2 .
2. $\lim_{N \rightarrow \infty} Q_N(f) = I(f)$ for every $f \in C(\mathbb{S}^2)$.
3. $\lim_{N \rightarrow \infty} Q_N(Y_{\ell, m}) = 0$ for all spherical harmonics $Y_{\ell, m}$ of degree $\ell \geq 1$ from a (real) $L_2(\mathbb{S}^2, \sigma_2)$ -orthonormal basis $\{Y_{\ell, m}\}$. (This is *Weyl's criterion* on the sphere.)
4. $\lim_{N \rightarrow \infty} D(Z_N; \mathbb{S}^2, \mathcal{C}) = 0$.

The spherical cap discrepancy can be estimated in terms of Weyl sums by means of *Erdős–Turán type inequalities*¹ (Grabner [19], also cf. Li and Vaaler [25])

¹ Such inequalities are a generalization of Erdős and Turán's result for the unit circle [16, 17].

$$D(Z_N; \mathbb{S}^2, \mathcal{C}) \leq \frac{c_1}{L+1} + \sum_{\ell=1}^L \left(\frac{c_2}{\ell} + \frac{c_3}{L+1} \right) \sum_{m=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=0}^{N-1} Y_{\ell,m}(\mathbf{x}_j) \right|,$$

where L is any positive integer and the positive constants c_1 , c_2 , and c_3 are independent of N , or *LeVeque type inequalities* ([29], generalizing LeVeques result for the unit circle [24])

$$\begin{aligned} c_4 \left[\sum_{\ell=1}^{\infty} a_{\ell} \sum_{m=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=0}^{N-1} Y_{\ell,m}(\mathbf{x}_j) \right|^2 \right]^{1/2} &\leq D(Z_N; \mathbb{S}^2, \mathcal{C}) \\ &\leq c_5 \left[\sum_{\ell=1}^{\infty} b_{\ell} \sum_{m=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=0}^{N-1} Y_{\ell,m}(\mathbf{x}_j) \right|^2 \right]^{1/(d+2)}, \end{aligned}$$

where $a_{\ell} := \Gamma(\ell - 1/2) / \Gamma(\ell + d + 1/2) \asymp 1/\ell^{d+1} =: b_{\ell}$, for some positive constants c_4 and c_5 which are independent of N . The integers

$$Z(d, 0) = 1, \quad Z(d, \ell) = (2\ell + d - 1) \frac{\Gamma(\ell + d - 1)}{\Gamma(d)\Gamma(\ell + 1)}$$

denote the number of linearly independent spherical harmonics $Y_{\ell,m}$ of degree ℓ .

Instead of using spherical caps as test sets, one can define discrepancy with respect to spherical rectangles (as done in this paper) or, as proposed by Sjögren [37], with respect to the family of so-called K -regular test sets. A σ_2 -measurable set $A \subseteq \mathbb{S}^2$ is defined to be K -regular if the σ_2 -measure of the δ -neighborhood (δ sufficiently small) of its boundary,

$$\{\mathbf{z} \in \mathbb{S}^2 : \text{dist}(A, \mathbf{z}) \leq \delta, \text{dist}(\mathbb{S}^2 \setminus A, \mathbf{z}) \leq \delta\}, \quad \text{dist}(A, \mathbf{z}) := \inf_{\mathbf{z}' \in A} \|\mathbf{z} - \mathbf{z}'\|,$$

is linearly bounded by $K \delta$. Clearly, spherical caps (rectangles) are K -regular for some $K > 0$. In [1] Andrievskii, Blatt and Götz related the discrepancy of a measure with the error in integration of polynomials in the following sense.

Proposition 1 *There exists a universal constant C_0 such that for every probability measure ν supported on \mathbb{S}^2 and every K -regular set $A \subseteq \mathbb{S}^2$ there holds*

$$|\nu(A) - \sigma_2(A)| \leq C_0 \inf_{n \in \mathbb{N}} \left\{ \frac{K}{n} + C(\nu, n) \right\},$$

where

$$C(v, n) := \sup \left\{ \left| \int p \, d\nu - \int p \, d\sigma_2 \right| : \begin{array}{l} p \text{ polynomial on } \mathbb{S}^2, \\ \deg p \leq qn, \, |p| \leq 1 \text{ on } \mathbb{S}^2 \end{array} \right\}$$

and $q = 3$.²

In particular, if ν is the counting measure $\frac{1}{N} \sum_{\mathbf{z} \in Z_N} \delta_{\mathbf{z}}$ induced by the node set Z_N of an equally weighted quadrature rule Q_N on \mathbb{S}^2 , then we have that

$$\begin{aligned} \nu(A) - \sigma_2(A) &= \frac{|Z_N \cap A|}{N} - \sigma_2(A), \\ &\times \int p \, d\nu - \int p \, d\sigma_2 = \frac{1}{N} \sum_{\mathbf{z} \in Z_N} p(\mathbf{z}) - \int p \, d\sigma_2 \end{aligned}$$

in Proposition 1.

Let $D(Z_N; \mathbb{S}^2, \mathcal{F}_K)$ denote the discrepancy with respect to the family of K -regular test sets and $D(Z_N; \mathbb{S}^2, \Omega)$ be the spherical rectangle discrepancy.

Theorem 2 *Let $\{Z_N\}$ be a sequence of N -point configurations with $N = b^m$, $m \geq 1$, defined by $(0, m, 2)$ -nets P_N in base b lifted to the sphere \mathbb{S}^2 by means of $Z_N = \Phi(P_N)$. Then the following holds:*

- (i) $\lim_{N \rightarrow \infty} D(Z_N; \mathbb{S}^2, \mathcal{F}_K) = 0$ for every fixed $K > 0$.
- (ii) $\lim_{N \rightarrow \infty} D(Z_N; \mathbb{S}^2, \mathcal{F}_K) = 0$.
- (iii) $\lim_{N \rightarrow \infty} D(Z_N; \mathbb{S}^2, \Omega) = 0$.

Consequently, the sequence $\{Z_N\}$ is asymptotically uniformly distributed on \mathbb{S}^2 .

Proof Let P_N be an $(0, m, 2)$ -net with $N = b^m$ points ($m \geq 1$) lifted to the sphere \mathbb{S}^2 and $\mathbf{z}_k = \Phi(\mathbf{x}_k)$ ($0 \leq k < N$). Then, using 'cylindrical' coordinates $\mathbf{z} = (\sqrt{1-t^2}\mathbf{z}^*, t)$, where $\mathbf{z}^* \in \mathbb{S}^1$ and $-1 \leq t \leq 1$, and the decomposition $d\sigma_2(\mathbf{z}) = (1/2) \, dt \, d\sigma_1(\mathbf{z}^*)$ ([28]), for every polynomial p on \mathbb{S}^2 (satisfying $|p(\mathbf{z})| \leq 1$ on \mathbb{S}^2) we get

$$\begin{aligned} Q_N(p) - I(p) &= \frac{1}{N} \sum_{k=0}^{N-1} p(\mathbf{z}_k) - \int_{\mathbb{S}^2} p \, d\sigma_2 \\ &= \int_{\mathbb{S}^1} \left[\frac{1}{N} \sum_{k=0}^{N-1} p(\mathbf{z}_k) - \frac{1}{2} \int_{-1}^1 p(\mathbf{z}) \, dt \right] d\sigma_1(\mathbf{z}^*). \end{aligned}$$

For each fixed $\mathbf{z}^* \in \mathbb{S}^1$ we define a new N -point configuration \widehat{Z}_N by aligning all points in Z_N such that they have the 'same \mathbf{z}^* ', that is $\widehat{\mathbf{z}}_k = (\sqrt{1-t_k^2}\mathbf{z}^*, t_k)$ ($0 \leq k < N$).

² Note that in [1] everything is done in \mathbb{R}^d .

Clearly, \widehat{Z}_N depends on \mathbf{z}^* . \widehat{Z}_N has N points, since the underlying system P_N is a $(0, m, 2)$ -net. Indicating the dependence on \mathbf{z}^* by $\widehat{\mathbf{z}}_k(\mathbf{z}^*)$ we write $Q_N(p) - I(p) = \Delta_1(p) + \Delta_2(p)$, where

$$\Delta_1(p) := \frac{1}{N} \sum_{k=0}^{N-1} p(\mathbf{z}_k) - \frac{1}{N} \sum_{k=0}^{N-1} \int_{\mathbb{S}^1} p(\widehat{\mathbf{z}}_k(\mathbf{z}^*)) \, d\sigma_1(\mathbf{z}^*),$$

$$\Delta_2(p) := \int_{\mathbb{S}^1} \left[\frac{1}{N} \sum_{k=0}^{N-1} p(\widehat{\mathbf{z}}_k(\mathbf{z}^*)) - \frac{1}{2} \int_{-1}^1 p(z) \, dt \right] d\sigma_1(\mathbf{z}^*).$$

First, we consider $\Delta_1(p)$. By definition of $(0, m, 2)$ -nets every elementary interval

$$[a/b^d, (a+1)/b^d) \times [a'/b^{m-d}, (a'+1)/b^{m-d}), \quad 0 \leq a < b^d, \quad 0 \leq a' < b^{m-d},$$

contains exactly one point of P_N . By construction of Z_N , the 2-sphere can be partitioned into $M \asymp \sqrt{N}$ polar zones A_1, \dots, A_M of equal sizes $1/\sqrt{N}$, each A_ℓ containing precisely $N_\ell \asymp \sqrt{N}$ points of Z_N ($N_1 + \dots + N_M = N$). Picking M heights τ_1, \dots, τ_M such that the circle C_ℓ with height τ_ℓ lies in A_ℓ , we move the points in A_ℓ on the circle C_ℓ giving them the same height τ_ℓ without changing the 'longitudes', that is $\mathbf{z}'_k := (\sqrt{1 - \tau_\ell^2} \mathbf{z}^*_k, \tau_\ell)$ for $\mathbf{z}_k = (\sqrt{1 - t_k^2} \mathbf{z}^*_k, t_k) \in A_\ell$. The error introduced in this way can be made arbitrarily small by increasing N , since the polynomial p is bounded and uniformly continuous on \mathbb{S}^2 and the widths of the polar zones uniformly decrease with increasing N . The integral $\int_{\mathbb{S}^1} p(\widehat{\mathbf{z}}_k(\mathbf{z}^*)) \, d\sigma_1(\mathbf{z}^*)$ averages the polynomial p over the circle on \mathbb{S}^2 with height t_k . In the zone A_ℓ we may use the approximation $\int_{\mathbb{S}^1} p((\sqrt{1 - \tau_\ell^2} \mathbf{z}^*, \tau_\ell)) \, d\sigma_1(\mathbf{z}^*)$. Therefore

$$\Delta_1(p) = \sum_{\ell=1}^M \frac{N_\ell}{N} \left[\frac{1}{N_\ell} \sum_{\mathbf{z}_k \in A_\ell} p(\mathbf{z}'_k) - \int_{\mathbb{S}^1} p((\sqrt{1 - \tau_\ell^2} \mathbf{z}^*, \tau_\ell)) \, d\sigma_1(\mathbf{z}^*) \right] + R_1(p),$$

where the error $R_1(p)$ goes to zero as $N \rightarrow \infty$. Observe, that the square-bracketed expression is the error of integration of an equally weighted quadrature rule on the circle C_ℓ with integration points \mathbf{z}'_k for $\mathbf{z}_k \in A_\ell$ induced by a horizontal strip of the underlying $(0, m, 2)$ -net P_N for the polynomial p restricted to C_ℓ . Since the extreme discrepancy of any $(0, m, 2)$ -net tends to zero as $m \rightarrow \infty$, it follows that the limit distribution of the integration nodes is given by σ_1 . Therefore the square-bracketed expression tends to zero uniformly for all $1 \leq \ell \leq M$ as $N \rightarrow \infty$.

Next, we consider $\Delta_2(p)$. We define the function $f(\mathbf{z}^*; t) := p((\sqrt{1 - t^2} \mathbf{z}^*, t))$ for $|t| \leq 1$ and each fixed $\mathbf{z}^* \in \mathbb{S}^1$, which is uniformly continuous and bounded in t and \mathbf{z}^* . Thus

$$\Delta_2(p) = \int_{\mathbb{S}^1} \left[\frac{1}{N} \sum_{k=0}^{N-1} f(\mathbf{z}^*; t_k) - \frac{1}{2} \int_{-1}^1 f(\mathbf{z}^*; t) \, dt \right] d\sigma_1(\mathbf{z}^*).$$

The square-bracketed expression is the error of integration for an equally weighted quadrature rule with integration nodes given by $t_k = 1 - 2x_k$, where the x_k 's are the 2nd-coordinates in the $(0, m, 2)$ -net P_N , integrating a function from the class $\{f(\mathbf{z}^*; \cdot) : \mathbf{z}^* \in \mathbb{S}^1\}$. We can apply Koksma's inequality and use that $|f(\mathbf{z}^*; t)| \leq 1$ to see that $\Delta_2(p) \rightarrow 0$ as $N \rightarrow \infty$. Thus, for every polynomial p on \mathbb{S}^2 (satisfying $|p(\mathbf{z})| \leq 1$ on \mathbb{S}^2) we get that $|\Delta(p)| \leq |\Delta_1(p)| + |\Delta_2(p)| \rightarrow 0$ as $N \rightarrow \infty$.

Now, we can apply Proposition 1. Let $q = 3$. Set $\nu_N = \frac{1}{N} \sum_{\mathbf{z} \in Z_N} \delta_{\mathbf{z}}$. Then to every $\varepsilon > 0$ we can choose a smallest integer n such that $K/n < \varepsilon/2$ and find an N_n such that $C(2, \nu_N, n) < \varepsilon/2$ for $N \geq N_n$ yielding

$$\left| \frac{|Z_N \cap A|}{N} - \sigma_2(A) \right| \leq C_0 \left\{ \frac{K}{n} + C(2, \nu_N, n) \right\} \leq C_0 \varepsilon,$$

which holds for every K -regular test set A (K is fixed). Item (i) follows.

Since spherical caps (rectangles) are K -regular (K' -regular) for some $K, K' > 0$, the Items (ii) and (iii) follow. By the list of equivalent characterizations of uniform distribution on \mathbb{S}^d , the sequence $\{Z_N\}$ is asymptotically uniformly distributed on \mathbb{S}^2 . \square

Concerning the convergence rate of the spherical cap discrepancy, it was an observation of Beck [4] that to any N -point set Z_N on \mathbb{S}^d there exists a spherical cap C such that

$$c_1 N^{-3/4} < \left| \frac{|Z_N \cap C|}{N} - \sigma_2(C) \right|$$

and (using probability arguments) there exist N -point sets Z_N on \mathbb{S}^2 such that

$$\left| \frac{|Z_N \cap C|}{N} - \sigma_2(C) \right| < c_2 N^{-3/4} \sqrt{\log N}$$

for any spherical cap C . (The numbers $c_i > 0$ are constants independent of N).

Remark 2 Thus, the correct order of decay (up to a $\sqrt{\log N}$ factor) of the spherical cap discrepancy of a sequence of low discrepancy N -point configurations on \mathbb{S}^2 is given by $N^{-3/4}$ as $N \rightarrow \infty$.

This is in contrast to the convergence rates (essentially [up to a logarithmic factor] $1/N$) given in Theorem 1 for the discrepancy with respect to spherical rectangles.

3 Numerical integration on \mathbb{S}^2

We consider now numerical integration of functions over \mathbb{S}^2 in some reproducing kernel Hilbert space defined on \mathbb{S}^2 . Let $\widehat{P}_k, k \in \mathbb{N}_0$, denote the Legendre polynomials. We define a reproducing kernel

$$K(\mathbf{z}, \mathbf{z}') = \sum_{\ell=0}^{\infty} \lambda_{\ell} \widehat{P}_{\ell}(\langle \mathbf{z}, \mathbf{z}' \rangle),$$

for some real numbers $\lambda_{\ell} \geq 0$. The rate of decay of λ_{ℓ} is related to the smoothness of the functions in the associated reproducing kernel Hilbert space. In particular, if $\lambda_{\ell} \asymp \ell^{-2s}$, then the reproducing kernel Hilbert space \mathcal{H}^s consists of functions with smoothness s , see [11] for more details.

In [11, Theorem 5.1] a choice of λ_{ℓ} was introduced for which $\lambda_{\ell} \asymp \ell^{-3}$ and for which the following reproducing kernel can be written explicitly as

$$K(\mathbf{z}, \mathbf{z}') = \sum_{\ell=0}^{\infty} \lambda_{\ell} \widehat{P}_{\ell}(\langle \mathbf{z}, \mathbf{z}' \rangle) = 2\mathcal{I} - \|\mathbf{z} - \mathbf{z}'\|,$$

where \mathcal{I} is the distance integral

$$\mathcal{I} = \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \|\mathbf{z} - \mathbf{z}'\| \, d\sigma_2(\mathbf{z}) d\sigma_2(\mathbf{z}').$$

This integral can be computed and has value $\mathcal{I} = 4/3$ (see [11]). The coefficients λ_{ℓ} are given by

$$\lambda_0 = \mathcal{I}, \quad \lambda_{\ell} = \mathcal{I} \frac{-(-1/2)_{\ell}}{(3/2)_{\ell}} \quad \text{for } \ell \geq 1,$$

where $(a)_{\ell} = a(a+1) \cdots (a+\ell-1) = \Gamma(a+\ell)/\Gamma(a)$ is the Pochhammer symbol. See [11] for more details.

The function $K(\mathbf{z}, \mathbf{z}')$ is a reproducing kernel of a Hilbert space $\mathcal{H}^{3/2}$ over \mathbb{S}^2 . In [11] it is shown that the squared worst-case error for numerical integration in this $\mathcal{H}^{3/2}$ is given by

$$e^2(Q_N, \mathcal{H}^{3/2}) = \mathcal{I} - \frac{1}{N^2} \sum_{k, \ell=0}^{N-1} \|\mathbf{z}_k - \mathbf{z}_{\ell}\|. \quad (6)$$

For quadrature rules Q_N with node sets maximizing the sum of distances $\sum_{k, \ell=0}^{N-1} \|\mathbf{z}_k - \mathbf{z}_{\ell}\|$ (that is, minimizing the right-hand side in (6) which in turn means that the nodes have minimal L_2 -discrepancy), it is known that there are constants $c, C > 0$ such that

$$c N^{-3/2} \leq e^2(Q_N, \mathcal{H}^{3/2}) \leq C N^{-3/2} \quad (7)$$

for N sufficiently large, see again [11, Corollary 5.2]. Note that the lower estimate always holds.

3.1 A lower bound on the worst-case error

Let Q_N^* be a quadrature rule whose integration points z_1^*, \dots, z_N^* maximize the sum of distances $\sum_{k,\ell=0}^{N-1} \|z_k - z_\ell\|$ or, equivalently, have minimal L_2 -discrepancy. (Such points always exist by the continuity of the distance function and compactness of the sphere). Then, using the lower bound in (7), we have

$$\begin{aligned} e^2(Q_N, \mathcal{H}^{3/2}) &= \mathcal{I} - \frac{1}{N^2} \sum_{k,\ell=0}^{N-1} \|z_k - z_\ell\| \geq \mathcal{I} - \frac{1}{N^2} \sum_{k,\ell=0}^{N-1} \|z_k^* - z_\ell^*\| \\ &= e^2(Q_N^*, \mathcal{H}^{3/2}) \geq c N^{-3/2} \end{aligned}$$

for some positive constant c not depending on N and N sufficiently large. Thus, one obtains that $e^2(Q_N, \mathcal{H}^{3/2}) \geq c N^{-3/2}$ for sufficiently large N for equal weight quadrature rule Q_N induced by any N -point configuration. This is in agreement with the results obtained in [22].

3.2 An upper bound on the worst-case error

By Stolarsky's invariance principle (3) and representation (6) we have

$$e^2(Q_N, \mathcal{H}^{3/2}) = \mathcal{I} - \frac{1}{N^2} \sum_{k,\ell=0}^{N-1} \|z_k - z_\ell\| = 4[D_2(Z_N; \mathbb{S}^2, \mathcal{C})]^2. \quad (8)$$

Since the spherical cap discrepancy provides an upper bound for the L_2 -discrepancy via $D_2(Z_N; \mathbb{S}^2, \mathcal{C}) \leq \sqrt{2}D(Z_N; \mathbb{S}^2, \mathcal{C})$, one has necessarily $e^2(Q_N, \mathcal{H}^{3/2}) \rightarrow 0$ as $N \rightarrow \infty$ for a sequence of asymptotically uniformly distributed N -point configurations on \mathbb{S}^2 . This applies in particular to digital nets on the sphere of the type considered in Theorem 2. A natural question is if such nets yield the same order of convergence as the worst-case error over the unit ball in $\mathcal{H}^{3/2}$ over \mathbb{S}^2 provided with the reproducing kernel $K(\mathbf{x}, \mathbf{y}) = (8/3) - \|\mathbf{x} - \mathbf{y}\|$ has [which is the same as of the optimal L_2 -discrepancy on \mathbb{S}^2 (see (8))] as suggested by the numerical results in Sect. 3.3.

Theorem 3 *Let $\{Z_N\}$ be a sequence of N -point configurations on \mathbb{S}^2 defined by point sets $P_N \subseteq [0, 1]^2$ lifted to the sphere \mathbb{S}^2 by means of $Z_N = \Phi(P_N)$. Then the equal weight quadrature rule Q_N associated with Z_N satisfies*

$$e^2(Q_N, \mathcal{H}^{3/2}) \leq \left(\frac{24}{\sqrt{3}} + 2\sqrt{2} \right) D^*(P_N; [0, 1]^2, \mathcal{R}^*).$$

Proof Notice that $\int_{\mathbb{S}^2} \|z - z'\| \, d\sigma_2(z')$ does not depend on $z \in \mathbb{S}^2$. Thus, defining the function

$$\Delta(\mathbf{w}) := \int_{\mathbb{S}^2} \|\mathbf{w} - z\| \, d\sigma_2(z) - \frac{1}{N} \sum_{k=0}^{N-1} \|\mathbf{w} - z_k\|, \quad \mathbf{w} \in \mathbb{S}^2, \quad (9)$$

one obtains

$$\begin{aligned} \frac{1}{N} \sum_{\ell=0}^{N-1} \Delta(z_\ell) &= \int \int_{\mathbb{S}^2} \|z - z'\| \, d\sigma_2(z) \, d\sigma_2(z') - \frac{1}{N^2} \sum_{k,\ell=0}^{N-1} \|z_k - z_\ell\| \\ &= e^2(Q_N, \mathcal{H}^{3/2}) \end{aligned}$$

and therefore

$$e^2(Q_N, \mathcal{H}^{3/2}) \leq \max_{0 \leq \ell < N} \Delta(z_\ell) \leq \sup_{z \in \mathbb{S}^2} \Delta(z).$$

Note that the sum in (9) can be seen as the potential (with respect to the distance kernel) of the discrete measure associated with Z_N at \mathbf{w} . Thus, $\Delta(z_\ell)$ gives the deviation from the leading term of the asymptotic expansion (as $N \rightarrow \infty$) of this potential at z_ℓ .

Let

$$g(\alpha, \tau) = \|\mathbf{w} - \Phi(\alpha, \tau)\|.$$

Since, by (5), the transformation Φ is area-preserving, it follows that

$$\int_{\mathbb{S}^2} \|\mathbf{w} - z\| \, d\sigma_2(z) = \int_0^1 \int_0^1 g(\alpha, \tau) \, d\alpha \, d\tau.$$

Thus, for any fixed $\mathbf{w} \in \mathbb{S}^2$, we can view $\Delta(\mathbf{w})$ as the integration error of integrating the function g using the points P_N . By the Koksma–Hlawka inequality, this integration error is bounded by the star-discrepancy $D^*(P_N; [0, 1]^2, \mathcal{R}^*)$ of P_N times the total variation of the function g in the sense of Hardy and Krause.

The variation of g in the sense of Vitali is given by

$$V^{(1,2)}(g) = \sup_{\mathcal{P}} \sum_{J \in \mathcal{P}} |\delta(g, J)|,$$

where the supremum is taken over all partitions of $[0, 1)^2$ into subintervals $J = [a_1, a_2) \times [b_1, b_2)$ and $\delta(g, J) = g(a_1, b_1) - g(a_1, b_2) - g(a_2, b_1) + g(a_2, b_2)$. The variation of the one-dimensional projections is given by

$$V^{(1)}(g) = \sup_{0=x_0 < x_1 < \dots < x_M=1} \sum_{k=1}^M |g(x_k, 1) - g(x_{k-1}, 1)|$$

and

$$V^{(2)}(g) = \sup_{0=y_0 < y_1 < \dots < y_M=1} \sum_{k=1}^M |g(1, y_k) - g(1, y_{k-1})|.$$

The total variation of g in the sense of Hardy and Krause is then given by

$$V(g) = V^{(1)}(g) + V^{(2)}(g) + V^{(1,2)}(g).$$

Let $\mathbf{w} = (0, 0, \pm 1)$. Then $\delta(g, J) = 0$ for all rectangles J and therefore $V^{(1,2)}(g) = 0$. Further, $\Phi(\alpha, 1) = (0, 0, -1)$ for all $0 \leq \alpha \leq 1$ and therefore $V^{(1)}(g) = 0$. Finally, $V^{(2)}(g) = |g(1, 0) - g(1, 1)| = 2$ because of the monotonicity of $g(1, \cdot)$. Thus we have $V(g) = 2$.

Let $\mathbf{w} \neq (0, 0, \pm 1)$. Then there are $u, v \in (0, 1)^2$ such that $\mathbf{w} = \Phi(u, v)$. Again, we have $V^{(1)}(g) = 0$. Further, we have $V^{(2)}(g) \leq 2\sqrt{2}$, where we have equality if $u = 1$ and $v = 1/2$.

Now we consider $V^{(1,2)}(g)$. The variation $V^{(1,2)}(g)$ does not change by changing u because of the rotational symmetry of g about the polar axis. We may therefore assume without loss of generality that $u = 1/2$. First, let $v = 1/2$. The mixed derivative

$$\frac{\partial^2 g}{\partial \alpha \partial \tau}(\alpha, \tau) = \frac{\partial^2 g}{\partial \tau \partial \alpha}(\alpha, \tau) = -4\pi \frac{(1-2\tau)(1+\sqrt{(1-\tau)\tau} \cos(2\pi\alpha)) \sin(2\pi\alpha)}{\sqrt{(1-\tau)\tau}(2+4\sqrt{(1-\tau)\tau} \cos(2\pi\alpha))^{3/2}}$$

is finite for $0 \leq \alpha \leq 1$ and $0 < \tau < 1$ with $\Phi(\alpha, \tau) \neq \mathbf{w}$. In particular, its sign does not change for (α, τ) in the interior of one of the four quadrants $\widehat{T}_1 = [0, 1/2] \times [0, 1/2]$, $\widehat{T}_2 = [0, 1/2] \times [1/2, 1]$, $\widehat{T}_3 = [1/2, 1] \times [0, 1/2]$, $\widehat{T}_4 = [1/2, 1] \times [1/2, 1]$ of the square. For a subinterval J with \overline{J} contained in the interior of one of these quadrants, one can use

$$\delta(g; J) = \int_J \frac{\partial^2 g}{\partial \alpha \partial \tau}(\mathbf{x}) \, d\mathbf{x} = \text{VOL}(J) \frac{\partial^2 g}{\partial \alpha \partial \tau}(\mathbf{x}_J) \quad \text{for some } \mathbf{x}_J \in \overline{J} \quad (10)$$

to determine the sign of $\delta(g; J)$. For a subinterval J which shares an upper or lower boundary with the square, the quantity $\delta(g; J)$ reduces to a difference of two function values, since g remains constant for $\tau = 0, 1$. In this case one can use monotonicity of the function g along horizontals (decreasing towards $\alpha = 1/2$). For \overline{J} with \mathbf{w} as one corner, one can still deduce if either $\delta(g; J) \leq 0$ or $\delta(g; J) \geq 0$. It suffices to consider partitions $\mathcal{P}_{\mathbf{w}}$ defined by horizontal and vertical lines including the lines with $\tau = 1/2$ and $\alpha = 1/2$. From our observations on the sign of $\delta(g; J)$ we conclude that the expression $\sum_{J \in \mathcal{P}_{\mathbf{w}}} |\delta(g; J)|$ can be reduced to two summands for each quadrant (and by symmetry)

$$\begin{aligned} V^{(1,2)}(g) = \sum_{J \in \mathcal{P}_w} |\delta(g, J)| = & -2(g(0, \Delta\tau') - g(1/2, \Delta\tau') + 0 - 2) \\ & + 2(g(0, \Delta\tau') - g(1/2, \Delta\tau')) \\ & + 2(2 - 0 + g(1/2, 1 - \Delta\tau'') - g(0, 1 - \Delta\tau'')) \\ & + 2(g(0, 1 - \Delta\tau'') - g(1/2, 1 - \Delta\tau'')), \end{aligned}$$

where $\Delta\tau'$ and $\Delta\tau''$ denote the “heights” of the first and last row of subintervals of \mathcal{P}_w .

Cancelling terms, we arrive at

$$V^{(1,2)}(g) = 8 \quad \text{for } (u, v) = (1/2, 1/2).$$

Therefore, for the case $v = 1/2$, we can use the Koksma–Hlawka inequality to obtain

$$|\Delta(\mathbf{w})| \leq D_N^*(P_N)V(g) \leq D_N^*(P_N)(8 + 2\sqrt{2}).$$

Now assume that $0 < v < 1/2$ (the case $1/2 < v < 1$ follows because of symmetry). Here, the mixed derivative is given by

$$\begin{aligned} \frac{\partial^2 g}{\partial \alpha \partial \tau}(\alpha, \tau) = \frac{\partial^2 g}{\partial \tau \partial \alpha}(\alpha, \tau) = & -16\pi(1-v)v(1-2\tau) \\ & \times R(\cos(2\pi\alpha)) \sin(2\pi\alpha)[g(\alpha, \tau)]^{-3}, \end{aligned}$$

where the linear form R is given by

$$R(x) = x + \frac{v - \tau + (1 - 2v)(1 - \tau)\tau}{\sqrt{(1 - v)v(1 - \tau)\tau(1 - 2\tau)}}.$$

Hence the mixed derivative is again finite for $0 \leq \alpha \leq 1$ and $0 < \tau < 1$ with $\Phi(\alpha, \tau) \neq \mathbf{w}$. Furthermore, it vanishes on the lines $\alpha = 0, 1$ and on the line $\alpha = 1/2$ (except when $\tau = 1/2$, where it is undefined). It does not vanish on the line $\tau = 1/2$. Finally, it vanishes on the set (cf. Fig. 1)

$$\Gamma := \{(\alpha, \tau) : (1 - 2\tau) R(\cos(2\pi\alpha)) = 0, 0 \leq \alpha \leq 1, 0 < \tau < 1\}.$$

(Note that the mixed derivative is singular everywhere along the lower and upper boundary of the unit square which are mapped to the poles of the sphere). The set Γ is symmetric in the sense that $(\alpha, \tau) \in \Gamma$ if and only if $(1 - \alpha, \tau) \in \Gamma$. From the observation

$$R(x)|_{\tau=v} = x + \frac{0 + (1 - 2v)(1 - v)v}{(1 - v)v(1 - 2v)} = x + 1$$

it follows that Γ and the line $\tau = v$ intersect only in the point $(1/2, v)$. We observe that the following three relations are equivalent:

$$\begin{aligned} |R(x) - x| &\leq 1, \\ (v - \tau)(v - 3v\tau + 3v\tau^2 - \tau^3) &\leq 0, \\ \tau &\geq v \quad \text{and} \quad \tau^3 + 3v\tau \leq 3v\tau^2 + v. \end{aligned}$$

From the last pair we obtain the equivalence

$$|R(x) - x| \leq 1 \quad \text{if and only if} \quad v \leq \tau \leq v + (1 - v)^{2/3}v^{1/3} - (1 - v)^{1/3}v^{2/3} =: \tau_v.$$

We conclude that Γ is the graph of a curve contained in the strip $v \leq \tau \leq \tau_v$ which is a function $\tau(\alpha)$ (assuming the value τ_v at $\alpha = 0, 1$ and v at $\alpha = 1/2$) and is a function $\alpha(\tau)$ when restricted to either the left or right half of the unit square. We record that $\tau_v < 1/2$ if $0 < v < 1/2$ and $\tau_v = 1/2$ if $v = 1/2$. Moreover, the vertical line test also shows that the function $\tau(\alpha)$ is strictly monotonically decreasing towards $\alpha = 1/2$. It is also continuous and continuously differentiable as can be seen from an implicit differentiation of $R(\cos(2\pi\alpha)) = 0$ (the factor $(1 - 2\tau)$ can not be zero in our setting):

$$\tau'(\alpha) = -4\pi \sin(2\pi\alpha) \frac{(1 - 2\tau)^2(1 - \tau)^2\tau\sqrt{(1 - v)v(1 - \tau)\tau}}{v - 3v\tau + 3v\tau^2 - \tau^3 + 3(\tau - v)(1 - \tau)\tau},$$

where $\tau = \tau(\alpha)$.

[The denominator is a strictly monotonically increasing function on the interval $(v, 1/2)$]. Using the relation $R(\cos(2\pi\alpha)) = 0$ along Γ in order to substitute $\cos(2\pi\alpha)$ in $g(\alpha, \tau)$, we obtain g restricted to Γ and its first derivative in the forms

$$g_\Gamma(\alpha) := g(\alpha, \tau(\alpha)) = 2\sqrt{\frac{\tau(\alpha) - v}{1 - 2v}}, \quad g'_\Gamma(\alpha) = \frac{2}{1 - 2v} \frac{\tau'(\alpha)}{g_\Gamma(\alpha)}.$$

Finally, we observe that g is decreasing along horizontal lines as α tends to $1/2$, since

$$\frac{\partial g}{\partial \alpha}(\alpha, \tau) = -8\pi\sqrt{(1 - v)v(1 - \tau)\tau} \frac{\sin(2\pi\alpha)}{g(\alpha, \tau)}, \quad (\alpha, \tau) \in [0, 1]^2, (\alpha, \tau) \neq (1/2, v)$$

and g is decreasing along vertical lines in the strip $v \leq \tau \leq 1/2$ as τ tends to v , since

$$\frac{\partial g}{\partial \tau}(\alpha, \tau) = 2 \frac{H(\cos(2\pi\alpha))}{g(\alpha, \tau)}, \quad H(x) = 1 - 2v + \sqrt{\frac{(1 - v)v}{(1 - \tau)\tau}}(1 - 2\tau)x.$$

Similar as in the case $v = 1/2$, the curve Γ and the vertical line $\alpha = 1/2$ divide the unit square into four regions T_1, T_2, T_3, T_4 . In the interior of each region the mixed derivative has the same sign. By (10), the sign of $\delta(g; J)$ is the same for all subintervals

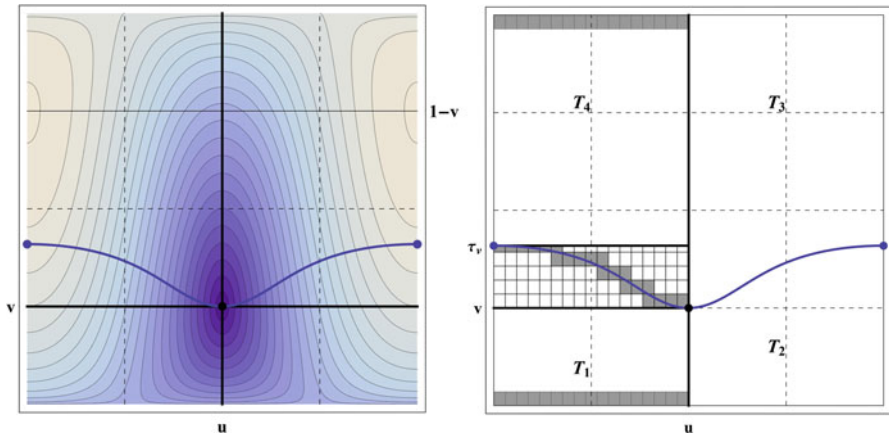


Fig. 1 Contour plot of $g(\alpha, \tau)$ with curve Γ and scheme to compute $V^{(1,2)}(g)$

contained in a fixed region T_k . Suppose \mathcal{P}_w is a partition of the unit square determined by a grid which is symmetric with respect to $\alpha = 1/2$ and also contains the vertical $\alpha = u (= 1/2)$ and the horizontals $\tau = v$ and $\tau = \tau_v$. (It suffices to consider this type of partitions.) The horizontals $\tau = v$ and $\tau = \tau_v$ subdivide the regions further into a rectangle T'_k without the curve Γ and a part T''_k with Γ as part of the boundary. By symmetry (cf. Fig. 1)

$$\begin{aligned} V^{(1,2)}(g) &= \sum_{J \in \mathcal{P}_w} |\delta(g, J)| = 2(g(0, \Delta\tau') - g(1/2, \Delta\tau')) - 2 \sum'_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T'_1}} \delta(g, J) \\ &\quad - 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T''_1, \\ J \cap \Gamma = \emptyset}} \delta(g, J) + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T'_1 \cup T''_4, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T''_4, \\ J \cap \Gamma = \emptyset}} \delta(g, J) \\ &\quad + 2 \sum'_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T'_4}} \delta(g, J) + 2(g(0, 1 - \Delta\tau'') - g(1/2, \Delta\tau'')), \end{aligned}$$

where $\Delta\tau'$ and $\Delta\tau''$ denote the “heights” of the first and last row of subintervals of \mathcal{P}_w and in the sums \sum' one excludes the J 's from the first and last row. Using cancellation at “interior” nodes, we obtain

$$\begin{aligned} V^{(1,2)}(g) &= 2(g(0, \Delta\tau') - g(1/2, \Delta\tau')) + 2(g(0, v) - 0 - g(0, \Delta\tau')) \\ &\quad + g(1/2, \Delta\tau') \end{aligned}$$

$$\begin{aligned}
& -2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq T_1'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_1} \cup \overline{T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_4}'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) \\
& + 2(g(0, 1 - \Delta\tau'') - g(1/2, \Delta\tau'')) \\
& + 2(g(0, \tau_v) - g(1/2, \tau_v) + g(1/2, 1 - \Delta\tau'') - g(0, 1 - \Delta\tau'')) \\
& = 2g(0, v) - 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_1}'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_1} \cup \overline{T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| + 2 \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_4}'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) \\
& + 2(g(0, \tau_v) - g(1/2, \tau_v)).
\end{aligned}$$

Let $v = y_m < y_{m+1} < \dots < y_{m+K+1} = \tau_v$ denote the τ -values of the grid defining \mathcal{P}_w in the strip $v \leq \tau \leq \tau_v$. To every y_{m+k} with $0 \leq k \leq K-1$ there exists a maximal $x_{\ell_{m+k}}$ of the α -values defining the grid such that the subinterval $[x_{\ell_{m+k-1}}, y_{m+k}) \times [x_{\ell_{m+k}}, y_{m+k+1})$ does not intersect Γ . For consistency reason we set $\ell_{m+K} = 0$, so that $x_{\ell_{m+K}} = 0$. Then

$$\begin{aligned}
- \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_1}'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) &= \sum_{k=0}^{K-1} (g(0, y_{m+k+1}) - g(x_{\ell_{m+k}}, y_{m+k+1})) \\
&+ g(x_{\ell_{m+k}}, y_{m+k}) - g(0, y_{m+k})) \\
&= g(0, y_{m+K}) - g(0, y_m) \\
&- \sum_{k=0}^{K-1} (g(x_{\ell_{m+k}}, y_{m+k+1}) - g(x_{\ell_{m+k}}, y_{m+k})).
\end{aligned}$$

Since g is decreasing along horizontals in the strip $v \leq \tau \leq 1/2$ as τ goes to v , one gets

$$- \sum_{\substack{J \in \mathcal{P}_w, \\ J \subseteq \overline{T_1}'', \\ J \cap \Gamma = \emptyset}} \delta(g, J) \leq g(0, y_{m+K}) - g(0, y_m) \leq g(0, \tau_v) - g(0, v).$$

Similarly, to every y_{m+k} with $1 \leq k \leq K$ there exists a minimal $x_{p_{m+k}}$ such that the subinterval $[x_{p_{m+k}}, y_{m+k}) \times [x_{p_{m+k+1}}, y_{m+k+1})$ does not intersect Γ . For consistency reason we set p_m to that index with $x_{p_m} = 1/2$. Then

$$\begin{aligned}
 \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_4}, \\ J \cap \Gamma = \emptyset}} \delta(g, J) &= \sum_{k=1}^K (g(x_{p_{m+k}}, y_{m+k}) - g(1/2, y_{m+k}) \\
 &\quad + g(1/2, y_{m+k+1}) - g(x_{p_{m+k}}, y_{m+k+1})) \\
 &= g(1/2, y_{m+K+1}) - g(1/2, y_{m+1}) \\
 &\quad - \sum_{k=1}^K (g(x_{p_{m+k}}, y_{m+k+1}) - g(x_{p_{m+k}}, y_{m+k})) \\
 &\leq g(1/2, y_{m+K+1}) - g(1/2, y_{m+1}) \leq g(1/2, y_{m+K+1}) = g(1/2, \tau_v).
 \end{aligned}$$

As an intermediate result we have

$$\begin{aligned}
 V^{(1,2)}(g) &\leq 2g(0, v) + 2(g(0, \tau_v) - g(0, v)) + 2 \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1 \cup T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| + 2g(1/2, \tau_v) \\
 &\quad + 2(g(0, \tau_v) - g(1/2, \tau_v)) = 4g(0, \tau_v) + 2 \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1 \cup T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)|.
 \end{aligned}$$

Using triangle inequality and monotonicity along horizontals we get

$$\begin{aligned}
 \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1 \cup T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| &= \sum_{k=0}^K \sum_{j=\ell_{m+k}}^{p_{m+k}-1} |g(x_j, y_{m+k}) - g(x_{j+1}, y_{m+k}) + g(x_{j+1}, y_{m+k+1}) \\
 &\quad - g(x_j, y_{m+k+1})| \leq \sum_{k=0}^K \sum_{j=\ell_{m+k}}^{p_{m+k}-1} (g(x_j, y_{m+k}) - g(x_{j+1}, y_{m+k})) \\
 &\quad + \sum_{k=0}^K \sum_{j=\ell_{m+k}}^{p_{m+k}-1} (g(x_j, y_{m+k+1}) - g(x_{j+1}, y_{m+k+1})) \\
 &= \sum_{k=0}^K (g(x_{\ell_{m+k}}, y_{m+k}) - g(x_{p_{m+k}}, y_{m+k})) + \sum_{k=0}^K (g(x_{\ell_{m+k}}, y_{m+k+1}) \\
 &\quad - g(x_{p_{m+k}}, y_{m+k+1})) \leq 2 \sum_{k=0}^K (g_{\Gamma}(x_{\ell_{m+k}}) - g_{\Gamma}(x_{p_{m+k}})).
 \end{aligned}$$

In the last step we used that the left side of a horizontal segment of successive rectangles of the covering of Γ is below and the right side is above the curve Γ by construction, cf. Fig. 1. Recall, that g_{Γ} is strictly monotonically decreasing as α tends to $1/2$. Since

$g_\Gamma(x_{\ell_{m+k-1}}) > g_\Gamma(x_{p_{m+k}})$ for $0 \leq k \leq K-1$ by monotonicity of g_Γ , we have

$$\begin{aligned} \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1} \cup \overline{T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| &\leq 2\{(g_\Gamma(x_{\ell_m}) - g_\Gamma(x_{p_m})) + \sum_{k=1}^K (g_\Gamma(x_{\ell_{m+k}}) - g_\Gamma(x_{\ell_{m+k-1}})) \\ &+ \sum_{k=1}^K (g_\Gamma(x_{\ell_{m+k-1}}) - g_\Gamma(x_{p_{m+k}}))\} = 2\{g_\Gamma(0) - g_\Gamma(1/2) \\ &+ \sum_{k=1}^K (g_\Gamma(x_{\ell_{m+k-1}}) - g_\Gamma(x_{p_{m+k}}))\}. \end{aligned}$$

By construction $x_{\ell_{m+K-1}} > x_{p_{m+K}} > x_{\ell_{m+K-2}} > x_{p_{m+K-1}} > \cdots > x_{\ell_{m+k}} > x_{p_m} = 1/2$. So, because of monotonicity of g_Γ , we increase the right-hand side of the estimate above when including terms for the gaps $[x_{p_{m+k}}, x_{\ell_{m+k-2}}]$. Thus

$$\sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1} \cup \overline{T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| \leq 4(g_\Gamma(0) - g_\Gamma(1/2)) = 4g_\Gamma(0),$$

where the expression in parentheses is the total variation of (monotone) one-dimensional function g_Γ restricted to $[0, 1/2]$. Putting everything together, we obtain

$$\begin{aligned} V^{(1,2)}(g) &\leq 4g(0, \tau_v) + 2 \sum_{\substack{J \in \mathcal{P}_{\mathbf{w}}, \\ J \subseteq \overline{T_1} \cup \overline{T_4}, \\ J \cap \Gamma \neq \emptyset}} |\delta(g, J)| \leq 4g(0, \tau_v) \\ &+ 8g_\Gamma(0) = 12g_\Gamma(0) = 24\sqrt{\frac{\tau_v - v}{1 - 2v}} \end{aligned}$$

It can be shown that the right-most side above as function of v is strictly monotonically increasing on $[0, 1/2]$ with

$$\lim_{v \rightarrow 1/2^-} \sqrt{\frac{\tau_v - v}{1 - 2v}} = \frac{1}{\sqrt{3}}.$$

We can use the Koksma–Hlawka inequality to obtain

$$|\Delta(\mathbf{w})| \leq D^*(P_N; [0, 1]^2, \mathcal{R}^*)V(g) \leq D^*(P_N; [0, 1]^2, \mathcal{R}^*) \left(\frac{24}{\sqrt{3}} + 2\sqrt{2} \right)$$

for $0 < v < 1/2$.

This concludes the proof. \square

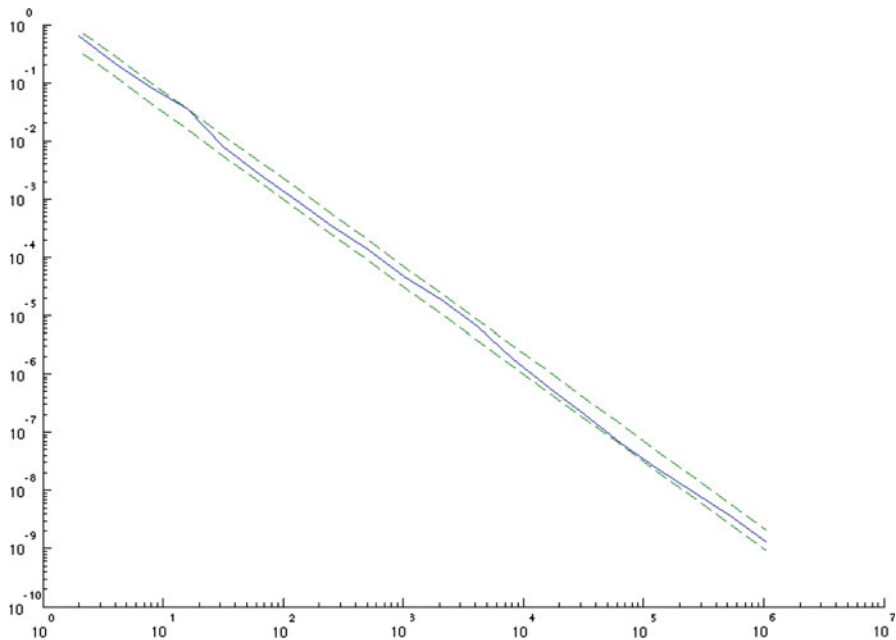


Fig. 2 The dashed lines show $N^{-3/2}$ and $(9/4)N^{-3/2}$, and the curve shows the squared worst-case error $e^2(Q_N, \mathcal{H}^{3/2})$, where the quadrature points are a digital net mapped to the sphere

Digital nets [15, 31] are explicit constructions of point sets in $[0, 1]^2$ with $D^*(P_N; [0, 1]^2, \mathcal{R}^*) = \mathcal{O}(N^{-1} \log N)$. By mapping them to the unit sphere \mathbb{S}^2 one also obtains explicit constructions of points on \mathbb{S}^2 with favorable discrepancy. We have the following corollary.

Corollary 1 *Let $b \geq 2$ and $m \geq 1$ be integers and let $N = b^m$. Let $\{Z_N\}$ be a sequence of N -point configurations on \mathbb{S}^2 defined by digital $(0, m, 2)$ -nets $P_N \in [0, 1]^2$ lifted to the sphere \mathbb{S}^2 by means of $Z_N = \Phi(P_N)$. Then the equal weight quadrature rules Q_N associated with Z_N satisfy*

$$e^2(Q_N, \mathcal{H}^{3/2}) = \mathcal{O}(N^{-1} \log N) \quad \text{as } N \rightarrow \infty.$$

3.3 Numerical results

We consider now the worst case error (6) for quadrature rules defined by digital nets based on a Sobol' sequence, see [39]. For efficient implementations of Sobol' sequences see [2, 8, 23]. Figure 2 shows the squared worst-case error $e^2(Q_N, \mathcal{H}^{3/2})$.

The numerical results suggest that the squared worst case error $e^2(Q_N, \mathcal{H}^{3/2})$ converges with order $\mathcal{O}(N^{-3/2})$ as $N \rightarrow \infty$.

Note that the first point of the Sobol' sequence (or any digital $(0, 2)$ -sequence for that matter) is always $(0, 0)$. Since $\Phi(0, 0) = (1, 0, 0)$, this point gets mapped to the North Pole. On the other hand, no point of the digital sequence gets mapped to the

Table 1 Numerical results: The worst-case error obtained when using digital nets over \mathbb{Z}_2 lifted to the sphere \mathbb{S}^2

m	$N = 2^m$	$e^2(Q_N, \mathcal{H}^{3/2})$	$N^{-3/2}$	$N^{3/2}e^2(Q_N, \mathcal{H}^{3/2})$
1	2	6.2622e-01	3.5355e-01	1.7712
2	4	2.1149e-01	1.2500e-01	1.6920
3	8	8.1448e-02	4.4194e-02	1.8430
4	16	3.5091e-02	1.5625e-02	2.2459
5	32	8.0526e-03	5.5242e-03	1.4577
6	64	2.6309e-03	1.9531e-03	1.3470
7	128	9.4336e-04	6.9053e-04	1.3661
8	256	3.4501e-04	2.4414e-04	1.4132
9	512	1.3374e-04	8.6316e-05	1.5495
10	1024	4.6029e-05	3.0517e-05	1.5083
11	2048	1.8846e-05	1.0789e-05	1.7468
12	4096	6.4670e-06	3.8146e-06	1.6953
13	8192	1.7873e-06	1.3486e-06	1.3252
14	16384	5.6815e-07	4.7683e-07	1.1915
15	32768	1.9912e-07	1.6858e-07	1.1811
16	65536	6.3194e-08	5.9604e-08	1.0602
17	131072	2.4122e-08	2.1073e-08	1.1447
18	262144	9.1906e-09	7.4505e-09	1.2335
19	524288	3.7001e-09	2.6341e-09	1.4047
20	1048576	1.3068e-09	9.3132e-10	1.4032

South Pole. This might not be a desirable feature. To remedy this situation one can randomize the $(0, 2)$ -sequence using a scrambling algorithm, see [27, 34]. In this case the sequence in $[0, 1]^2$ is still a $(0, 2)$ -sequence, but the point $(0, 0)$ only occurs with probability 0. Numerical investigation of scrambled Sobol' sequences yield similar results as the one shown in Fig. 2.

The numerical results lead us to the following conjecture.

Conjecture 1 Let $\mathbf{x}_0, \mathbf{x}_1, \dots \in [0, 1)^2$ be a $(0, 2)$ -sequence and let $\mathbf{z}_0, \mathbf{z}_1, \dots \in \mathbb{S}^2$ be the corresponding points on the sphere obtained by using the mapping Φ . Let $Q_N(f) = \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{z}_n)$. Then we have

$$e^2(Q_N, \mathcal{H}^{3/2}) = \mathcal{O}(N^{-3/2}) \quad \text{as } N \rightarrow \infty.$$

In other words, a $(0, 2)$ -sequence lifted to the 2-sphere via the mapping Φ achieves the optimal rate of convergence of the worst-case integration error in $\mathcal{H}^{3/2}$. By Stolarsky's invariance principle, the conjecture also implies that a $(0, 2)$ -sequence lifted to the 2-sphere via the mapping Φ achieves the optimal rate of decay of the spherical cap L_2 -discrepancy (Table 1).

Acknowledgments The first author is grateful to the School of Mathematics and Statistics at UNSW for their support.

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