Discrepancy, separation and Riesz energy of point sets on the unit sphere

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Abstract

When does a sequence of spherical codes with "good" spherical cap discrepancy, and "good" separation also have "good" Riesz s-energy?

For $d \geqslant 2$ and the Riesz s-energy for $0 < s < d$, we consider asymptotically equidistributed sequences of $\mathbb{S}^d$ codes with an upper bound δ on discrepancy and a lower bound Δ on separation. For such sequences, the difference between the normalized Riesz s-energy and the normalized energy double integral is bounded above by $\mathrm{O}\left(\delta^{1-s/d}\,\Delta^{-s}\,N^{-s/d}\right)$, where N is the number of code points. For well separated sequences of spherical codes, this bound becomes $\mathrm{O}\left(\delta^{1-s/d}\right)$.

We apply these bounds to minimum energy sequences, sequences of well-separated spherical designs, sequences of extremal fundamental systems, and sequences of equal area points.
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1 Introduction and Main Results

We consider the unit sphere $\mathbb{S}^d := \left\{x \in \mathbb{R}^{d+1} \mid \|x\| = 1\right\}$, for $d \geqslant 2$, and call a finite set of points of $\mathbb{S}^d$ a *spherical code*. There is a continuing interest in the generation and use of spherical codes which are in some sense well distributed, and the properties which can be used to distinguish better distributed codes from more poorly distributed ones. This paper examines the relationship between three such properties of sequences of spherical codes $\mathcal{X} := (X_1, X_2, \ldots)$, with

$$X_\ell := \{x_{\ell,1}, \ldots, x_{\ell,N_\ell}\} \subset \mathbb{S}^d.$$

These properties are the Riesz s-energy, the spherical cap discrepancy, and the separation of code points. It is known that a sequence of spherical codes with minimal Riesz s-energy and increasing numbers of points has "good" spherical cap discrepancy, and "good" separation, in a sense which is made more precise below. The question addressed in this paper concerns a partial converse to this result:

> When does a sequence of spherical codes with "good" spherical cap discrepancy, and "good" separation also have "good" Riesz s-energy?

The following definitions make these concepts more precise.

The normalized *Riesz s-energy* of a spherical code X is defined as $\mathrm{E}(X)\,U_s$, where $U_s(r) := r^{-s}$, the Riesz potential function, and $\mathrm{E}(X)$ is the normalized discrete energy functional

$$\mathrm{E}(X)\,u := \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} u\left(\|x - y\|\right).$$

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We also consider the corresponding normalized continuous energy functional, which is given by the double integral

$$\mathcal{I}\, u := \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} u\left(\|x-y\|\right) d\sigma(x)\, d\sigma(y),$$

where σ is the spherical probability measure, the uniform measure on $\mathbb{S}^d$ normalized so that $\sigma(\mathbb{S}^d) = 1$. It is well known that for $0 < s < d$, the normalized energy double integral of U_s has the value

$$\mathcal{I}\, U_s = 2^{d-s-1} \frac{\Gamma\left((d+1)/2\right) \Gamma\left((d-s)/2\right)}{\sqrt{\pi}\, \Gamma(d-s/2)}. \tag{1}$$

The normalized *spherical cap discrepancy* of a spherical code is the supremum over all spherical caps of the difference between the normalized area of the cap and the proportion of code points which lie in the cap. In other words, for $y \in \mathbb{S}^d, r \in (0,2]$, let $S(y,r)$ be the closed spherical cap $\{x \mid \|x-y\| \leqslant r\}$, and let σ_X be the normalized counting measure defined for $Y \in \mathbb{S}^d$ by

$$\sigma_X(Y) := \frac{|X \cap Y|}{|X|}.$$

Then the normalized spherical cap discrepancy of X is

$$\operatorname{disc}(X) := \sup_{y \in \mathbb{S}^d, r \in (0,2]} |\sigma\left(S(y,r)\right) - \sigma_X\left(S(y,r)\right)|.$$

We consider sequences $\mathcal{X}$ of spherical codes which are *asymptotically equidistributed* [6, Remark 4, p. 236], in the sense that the normalized spherical cap discrepancy is bounded above by a positive decreasing function $\delta : \mathbb{N} \to (0,2]$, with $\delta(N) \to 0$ as $N \to \infty$. Specifically,

$$\operatorname{disc}(X_\ell) < \delta(N_\ell). \tag{2}$$

We consider sequences $\mathcal{X}$ of spherical codes such that the minimum distance between code points is bounded below by a positive decreasing function $\Delta : \mathbb{N} \to (0,2]$, specifically,

$$\|x-y\| > \Delta(N_\ell) \tag{3}$$

for all $x, y \in X_\ell$.

An easy area argument shows that the order of the lower bound $\Delta(N)$ for the separation of the solution of the Tammes problem [32], the sequence which has the largest separation for each N, is $\Omega(N^{-1/d})$ [27, Theorem 2]. Therefore, for all sequences of $\mathbb{S}^d$ codes, $\Delta(N)N^{1/d}$ is bounded above by a constant, that is, $\Delta(N)N^{1/d}$ is of order at most $\mathrm{O}(1)$.

A sequence $\mathcal{X}$ of $\mathbb{S}^d$ codes is called *well separated* if there exists a constant $\gamma > 0$ such that we can set $\Delta(N) = \gamma N^{-1/d}$.

With these definitions in hand, we define an *admissible sequence* of spherical codes to be a triple $(\mathcal{X}, \delta, \Delta)$ such that (2) and (3) are satisfied. We can now state our main result.

Theorem 1. *For an admissible sequence $(\mathcal{X}, \delta, \Delta)$ of $\mathbb{S}^d$ spherical codes, the normalized Riesz s-energy for $0 < s < d$ is bounded by*

$$\left(\mathrm{E}(X_\ell) - \mathcal{I}\right) U_s = \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\, \Delta(N_\ell)^{-s}\, N_\ell^{-s/d}\right), \tag{4}$$

$$\left(\mathcal{I} - \mathrm{E}(X_\ell)\right) U_s = \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\right). \tag{5}$$

This result immediately implies the following.

Corollary 2. *For a well separated admissible sequence $(\mathcal{X}, \delta, \Delta)$ of $\mathbb{S}^d$ spherical codes, the normalized Riesz s-energy for $0 < s < d$ can be estimated by*

$$\mathrm{E}(X_\ell)\, U_s = \mathcal{I}\, U_s + \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\right). \tag{6}$$

Remarks

Measures with bounded density

Götz obtains a result [12, Proposition 13] similar to Corollary 2, that is, an estimate of Riesz energy in terms of ball discrepancy, but his result is for the difference in energy double integral between two probability measures satisfying a density bound [12, (12)], and so the result does not apply in our case. It is interesting to note, though, that if we set $\beta = d$ in [12, (12)], then the energy difference given by [12, Proposition 13] is also bounded by $C\,\delta^{1-s/d}$, where in this case δ is the discrepancy between the two probability measures.

Asymptotic equidistribution and weak-star convergence

It has long been known that such a sequence $\mathcal{X}$ of spherical codes is asymptotically equidistributed if and only if it is weak-star convergent, i.e. the corresponding sequence (σ_{X_ℓ}) of normalized counting measures converges weakly to σ,

$$\int_{\mathbb{S}^d} f(x)\, d\sigma_{X_\ell}(x) := \frac{1}{N_\ell} \sum_{x \in X_\ell} f(x) \to \int_{\mathbb{S}^d} f(x)\, d\sigma(x)$$

as $\ell \to \infty$ for all continuous $f : \mathbb{S}^d \to \mathbb{R}$.

Theorem 4.1 of R. Ranga Rao [28, p. 665] states that given a measure μ on $\mathbb{R}^{d+1}$ such that $\mu\mathcal{L}^{-1}$ is continuous for every linear function $\mathcal{L}$ on $\mathbb{R}^{d+1}$, a sequence of measures converges weakly to μ if and only if it converges to μ for certain discrepancies defined on half spaces. This theorem can be used to show that a sequence of $\mathbb{S}^d$ codes is weak-star convergent if and only if it converges to zero in normalized spherical cap discrepancy. Brauchart proves this equivalence relationship in another way in his Diplomarbeit [3], by appealing to Grabner's [13] Erdös-Turán inequality on the sphere.

Bounds in the best case

For any sequence of spherical codes, the normalized spherical cap discrepancy is bounded below such that $\delta(N_\ell) = \Omega\left(N_\ell^{-1/2-1/2d}\right)$, as stated by Beck [2, p. 10]. Thus, for a well separated sequence with the best possible normalized spherical cap discrepancy the estimate (6) gives an upper bound for the normalized Riesz s-energy of no better than

$$\mathrm{E}(X_\ell)\, U_s - \mathcal{I}\, U_s \leqslant \mathrm{O}\left(N_\ell^{(s-d)(d+1)/(2d^2)}\right).$$

In contrast, the best known upper bound for $\mathrm{E}(X_N)\, U_s - \mathcal{I}\, U_s$ for a minimum s-energy sequence $\varOmega_s$, for $d \geqslant 2$ and $s \in (0, d)$, is

$$\mathrm{E}(\varOmega_{s,N})\, U_s - \mathcal{I}\, U_s \leqslant -cN^{s/d-1}, \text{ with } c > 0, \tag{7}$$

as given by Kuijlaars and Saff [19, (1.6)].

2 Applications of Theorem 1

It is known that the following sequences of spherical codes are admissible.

1. Minimum energy sequences.

   See Section 3.

2. Well-separated sequences of spherical designs.

   See Section 4.

3. Sequences of extremal fundamental systems.

   Let $\{p_1, \ldots, p_{D_t}\}$ be a basis for the spherical polynomials of degree at most t. An *extremal fundamental system* is a spherical code X which maximizes the determinant $\det A(X)$, where A is the interpolation matrix of size $D_t \times D_t$ with entries $A_{i,j} := p_i(x_j)$. See [29, 31] for details.

   A sequence Ξ of extremal fundamental systems with increasing degree t is known to be well separated [29]. Marzo and Ortega-Cerdà [24] have recently shown that Ξ is asymptotically equidistributed. Corollary 2 therefore implies that the normalized Riesz s-energy of Ξ converges to the normalized energy double integral for all $s \in (0, d)$.

4. Well-separated, diameter-bounded equal area sequences.

   The sequence $\mathrm{EQP}(d)$ of recursive zonal equal area spherical codes, as described in the author's PhD thesis [23, 4.1], and implemented in the EQSP Matlab toolbox [22] is well separated [23, Theorem 4.3.2] and has normalized spherical cap discrepancy $\mathrm{disc}\big(\mathrm{EQP}(d, N)\big) = \mathrm{O}(N^{-1/d})$ [23, Theorem 5.4.1]. Our estimate (6) therefore yields the normalized energy estimate

$$\mathrm{E}(\mathrm{EQP}(d, N))\, U_s = \mathcal{I}\, U_s + \mathrm{O}\left(N^{(s-d)/d^2}\right).$$

   See [23, Section 5.4].

3 Minimum energy sequences

Minimum Riesz s-energy

For $q > 0$, let $\Omega_q = (\Omega_{q,1}, \Omega_{q,2}, \ldots)$ be a sequence of $\mathbb{S}^d$ codes such that $|\Omega_{q,N}| = N$ and such that $\Omega_{q,N}$ has the minimum Riesz q-energy for any $\mathbb{S}^d$ code with N code points.

It is known that for $q \in (0, d)$, Ω_q is asymptotically equidistributed [21, Chapter 2, 12, pp. 160–162] [6, Theorem 3, p. 236] [15, Theorem 1.1 p. 176]. Brauchart [4, Theorem 2.2, p. 24] gives a bound for the normalized spherical cap discrepancy of Ω_q of

$$\mathrm{disc}(\Omega_{q,N}) = \mathrm{O}(N^{-\alpha/d}). \tag{8}$$

where $\alpha := (d - q)/(d - q + 2)$.

For $q \in (d - 2, d)$, Ω_q is also known to be well separated [10, Theorem 1.5, p. 143]. Therefore, for $q \in (d - 2, d)$ and $s \in (0, d)$, Corollary 2 implies that $\mathrm{E}(\Omega_{q,N})\, U_s \to \mathcal{I}\, U_s$ as $N \to \infty$. Using Brauchart's bound (8) we obtain, for this case, the estimate

$$\mathrm{E}(\Omega_{q,N})\, U_s = \mathcal{I}\, U_s + \mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right) = \mathcal{I}\, U_s + \mathrm{O}\left(N^{-(1-s/d)(1-q/d)/(d-q+2)}\right).$$

For general $q > 0$, the situation is more complicated, and the known results on discrepancy and separation split into a number of cases. Let $\phi_{q,s}(N)$ be the order in N of the upper bound on $\mathrm{E}(\Omega_{q,N})\, U_s - \mathcal{I}\, U_s$ given by (4) above, given the currently known values of the bounds $\delta(N)$ and $\Delta(N)$ for Ω_q. Table 1 lists these results, giving references.

The result for $q = d$ in Table 1 is peculiar. The upper bound

$$\phi_{d,s}(N) = (\log N)^{(3s/d-1)/2}\, (\log \log N)^{(1-s/d)/2}$$

decreases to 0 as $N \to \infty$ when $s < d/3$, but increases when $s \geqslant d/3$. Kuijlaars and Saff comment that the order of the separation bound $\Delta(N)$ for Ω_d "most likely is not best possible" [19, p. 525]. This seems reasonable, since both $\Omega_{d+\epsilon}$ and $\Omega_{d-\epsilon}$ are known to be well separated.

The result for $q \in (0, d - 2)$ in Table 1 is also remarkable. The exponent

$$f(d, q, s) := -(1 - s/d)(d - q)/(d - q + 2)/d - s/d + s/(q + 2)$$

q	$\delta(N)$	$\Delta(N)$	$\phi_{q,s}(N)$
$(0, d-2]$ $(d \geqslant 3)$	$\mathrm{O}(N^{-\alpha/d})$ $[4, Ch.2]$	$\Omega(N^{-1/(q+2)})$ $[8, Th.3.5]$	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d-s/d+s/(q+2)}\right)$
$(d-2, d-1)$	$\mathrm{O}(N^{-\alpha/d})$ $[4, Ch.2]$	$\Omega(N^{-1/d})$ $[10, Th.1.5]$	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right)$
$d-1$	$\mathrm{O}(N^{-1/d}\log N)$ $[11, Th.4]$	$\Omega(N^{-1/d})$ $[11, Th.3]$	$\mathrm{O}\left(N^{-(1-s/d)/d}(\log N)^{-(1-s/d)}\right)$
$(d-1, d)$	$\mathrm{O}(N^{-\alpha/d})$ $[4, Ch.2]$	$\Omega(N^{-1/d})$ $[20, Th.8]$	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right)$
d	$\mathrm{O}\left(\sqrt{\frac{\log\log N}{\log N}}\right)$ $[7, Th.1]$	$\Omega\left((N\log N)^{-1/d}\right)$ $[19, (1.13)]$	$\mathrm{O}\left((\log N)^{(3s/d-1)/2}\,(\log\log N)^{(1-s/d)/2}\right)$
(d, ∞)	$\to 0$ $[15, Th.2.2]$	$\Omega(N^{-1/d})$ $[19, (1.12)]$	$\to 0$

Table 1: Discrepancy, separation and s-energy bounds for minimum q-energy sequences

is not always negative. In particular for $\phi_{s,s}(N)$, the upper bound from (4) for the normalized Riesz s-energy of the optimal Riesz s-energy points, the exponent $f(d,s,s)$ is not always negative:

$$\begin{aligned} f(d,s,s) &= -(1-s/d)(d-s)/(d-s+2)/d - s/d + s/(s+2) \\ &= \frac{(d-1)s^3 + (-2d^2+2d-2)s^2 + (d^3-d^2)s - 2d^2}{d^2\,(s+2)\,(d-s+2)}. \end{aligned}$$

For $d \geqslant 5$, $f(d,s,s)$ takes on positive values for s in some interval within $(0, d-2)$. For example, $f(5,s,s) > 0$ for $s \in (4-\sqrt{11}, 5/2)$, and our upper bound therefore diverges for this range of s.

In fact, our upper bound $\phi_{s,s}(N)$ is never tight for any $s \in (0,d)$, since it is always positive, and the best known upper bound for $\mathrm{E}(\varOmega_{s,N})\,U_s - \mathcal{I}\,U_s$ is given by (7), which is negative.

Minimum logarithmic energy

For $d \geqslant 2$, the normalized *logarithmic energy* of a spherical code X is given by $\mathrm{E}(X)\,U_{\log}$, where $U_{\log}(r) := -\log(r)$ is the logarithmic potential function. Let $\varOmega_{\log}$ be a sequence of $\mathbb{S}^d$ codes with such that $|\varOmega_{\log,N}| = N$ and such that $\varOmega_{\log,N}$ has the minimum normalized logarithmic energy for any $\mathbb{S}^d$ code with N code points.

The best known bound on the normalized spherical cap discrepancy $\mathrm{disc}(\varOmega_{\log,N})$ is Brauchart's bound, $\mathrm{O}(N^{-1/(d+2)})$ [5, Theorem 1.6]. For $d = 2$, the logarithmic energy points are also known to be well-separated [26, Theorem 1]. In this case, our estimate (6) implies the normalized energy estimate

$$\mathrm{E}(\varOmega_{\log,N})\,U_s = \mathcal{I}\,U_s + \mathrm{O}\left(N^{-(1-s/2)/4}\right)$$

for $s \in (0,2)$.

4 Well-separated sequences of spherical designs

A spherical t-design is a spherical code such that the corresponding normalized counting measure gives an equal weight quadrature functional which exactly integrates all spherical polynomials of degree to and including t [9]. In [17] it was proved that for a well separated sequence of spherical designs on $\mathbb{S}^2$ such that each t-design has $(t+1)^2$ points, the normalized Coulomb energy (i.e. Riesz 1-energy) has the same first term and a second term of the same order as the minimum normalized Coulomb energy for $\mathbb{S}^2$ codes.

The proof in [17] was the joint work of Hesse and the author, based on a problem posed by Sloan. Hesse [16] generalized the results of [17] to cover the Riesz s-energy for $0 < s < 2$.

To compare the results of [17] and [16] to energy bounds of the type treated here, we need a variant of Corollary 2.

From [13, Theorem 1] [14, (2.1)] we know that there is a constant C_G such that for any spherical t-design X_t on $\mathbb{S}^2$, we have

$$\operatorname{disc}(X_t) \leqslant \frac{C_G}{t+1}. \tag{9}$$

We therefore need to modify Corollary 2 to treat sequences $\mathcal{X}$ of spherical codes with normalized spherical cap discrepancy bounded by

$$\operatorname{disc}(X_\ell) < \delta(\ell). \tag{10}$$

Corollary 3. *For a well separated sequence $\mathcal{X}$ of $\mathbb{S}^d$ spherical codes, with normalized spherical cap discrepancy bounded by (10) the normalized Riesz s-energy for $0 < s < d$ can be estimated by*

$$\mathrm{E}(X_\ell)\, U_s = \mathcal{I}\, U_s + \mathrm{O}\left(\delta(\ell)^{1-s/d}\right). \tag{11}$$

We define a well separated admissible sequence of $\mathbb{S}^d$ designs to be the pair $(\mathcal{X}, \gamma)$, where $\mathcal{X} = (X_1, X_2, \ldots)$, with each spherical design X_t having strength t, and where $\mathcal{X}$ is well separated with separation constant γ.

We can now compare the results of [17] and [16] with the result obtained by combining the estimate (11) with the bound (9) on the normalized spherical cap discrepancy of spherical designs.

First we restate the main results from [17] with notation adjusted to match this paper, and recall from (1) the well known result that $\mathcal{I}\, U_1 = 1$.

Theorem 4. *Let $(\mathcal{X}, \gamma)$ be a well separated admissible sequence of $\mathbb{S}^2$ designs. Then the normalized Coulomb energy $\mathrm{E}(X_t)\, U_1$ of each spherical design $X_t \in \mathcal{X}$ of cardinality N_t is bounded above by*

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + C_\gamma\, (t+1)^{-3/2}\, N_t^{1/4} - \frac{1}{2}\,\frac{1}{t+3/2} - \frac{1}{2}\,\frac{(t+1)(t+2)}{t+3/2}\, N_t^{-1}.$$

The constant $C_\gamma \geqslant 0$ depends on the separation constant γ, but is independent of t.

Theorem 5. *Let $(\mathcal{X}, \gamma)$ be a well separated admissible sequence of $\mathbb{S}^2$ designs such that for some positive constant μ, $|X_t| = N_t \leqslant \mu(t+1)^2$. Then the normalized Coulomb energy of each $X_t \in \mathcal{X}$ is bounded above by*

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + C_{(\gamma,\mu)}\, N_t^{-1/2},$$

where $C_{(\gamma,\mu)} \geqslant 0$ is independent of t.

It is not yet known whether an infinite sequence of spherical designs exists which satisfies the premise of Theorem 5. If such a sequence $\mathcal{X}$ exists, Theorem 5 implies that its normalized Coulomb energy converges to the corresponding normalized energy double integral at the rate of $\mathrm{O}(t^{-1})$, that is

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + \mathrm{O}(t^{-1}).$$

Applying our estimate (11) and the bound (9) to a well separated admissible sequence $\mathcal{X}$ of spherical designs on $\mathbb{S}^2$, we obtain

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + \mathrm{O}(t^{-1/2}).$$

This is a slower rate of convergence than predicted by Theorem 5, but the result does not depend on the relationship between cardinality and strength required by Theorem 5.

If we use Theorem 4 with the sequence of spherical designs on $\mathbb{S}^2$ with the lowest known cardinality, that of [18, Theorem 2.3], which has cardinality of $\mathrm{O}(t^3)$, we obtain

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + \mathrm{O}(t^{-3/4}).$$

This assumes that the sequence of [18, Theorem 2.3] is well separated. From the construction given in [18, Section 5], this assumption seems reasonable. Thus Theorem 4 gives a faster rate of convergence for this sequence than is predicted by Corollary 3.

If instead of the normalized Coulomb energy, we use the normalized Riesz s energy for $s \in (0, 2)$, then for a well admissible separated sequence $\mathcal{X}$ of spherical designs on $\mathbb{S}^2$, the estimate (11) and the bound (9) yield

$$\mathrm{E}(X_t)\, U_s \leqslant \mathcal{I}\, U_s + \mathrm{O}\left(t^{s/2-1}\right). \tag{12}$$

Hesse's result [16, Theorem 2] implies that for a sequence $\mathcal{X}$ of spherical designs which satisfies the premise of Theorem 5, the Riesz s for $s \in (0, 2)$ is bounded as

$$\mathrm{E}(X_t)\, U_s \leqslant \mathcal{I}\, U_s + \mathrm{O}\left(t^{s-2}\right).$$

Again, this result is better than our corresponding result (12).

5 Preliminary lemmas

Our proof of Theorem 1 needs a a few well known results, which we state here as lemmas.

Lemma 6. *The Lebesgue area measure of the sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ is given by*

$$\omega_d := \omega_d(\mathbb{S}^d) = \frac{2\pi^{\frac{d+1}{2}}}{\Gamma(\frac{d+1}{2})}.$$

Remarks. This usage of ω_d agrees with Müller [25] and Reimer [30], but not with Landkof [21, Chapter 1, 2, p. 45] or Andrews, Askey and Roy [1, Section 9.6, p. 455], who would put ω_{d+1} where we have ω_d.

Lemma 7. *For $R \in (0, 2]$ and any $x \in \mathbb{S}^d$, the normalized area integral $\mathcal{V}_d(R) := \sigma\left(S(x, R)\right)$ can be evaluated by*

$$\mathcal{V}_d(R) = \frac{\omega_{d-1}}{\omega_d} \int_0^R r^{d-1} \left(1 - \frac{r^2}{4}\right)^{\frac{d}{2}-1} dr,$$

independent of the point x, and the derivative $D\mathcal{V}_d$ is given by

$$D\mathcal{V}_d(R) = \frac{\omega_{d-1}}{\omega_d} R^{d-1} \left(1 - \frac{R^2}{4}\right)^{\frac{d}{2}-1},$$

where the limit for the derivative is defined from above at 0, and from below at 2.

Lemma 8. *For $R \in (0, T]$, $T \in (0, 2]$ the normalized area integral $\mathcal{V}_d(R)$ can be estimated by*

$$\mathcal{V}_d(R) \in \big[C_{L,d}(T), C_{H,d}\big)\, \frac{R^d}{d},$$

where

$$C_{L,d}(T) := \left(1 - \frac{T^2}{4}\right)^{\frac{d}{2}-1} C_{H,d}, \quad C_{H,d} := \frac{\omega_{d-1}}{\omega_d}. \tag{13}$$

Lemma 9. *For $R \in (0, 2]$ and any $x \in \mathbb{S}^d$, for any integrable function $u : (0, 2] \to \mathbb{R}$, the single integral*

$$\mathcal{J}_d(x; R)\, u := \int_{\|x-y\| \leqslant R} u(\|x - y\|)\, d\sigma(y)$$

can be evaluated by

$$\begin{aligned} \mathcal{J}_d(x; R)\, u = \mathcal{J}_d(R)\, u &= \int_0^R u(r) d\mathcal{V}_d(r) \\ &= \frac{\omega_{d-1}}{\omega_d} \int_0^R u(r)\, r^{d-1} \left(1 - \frac{r^2}{4}\right)^{\frac{d}{2}-1} dr, \end{aligned} \tag{14}$$

which is independent of x.

Corollary 10. *For any integrable function $u : (0, 2] \to \mathbb{R}$, the double integral $\mathcal{I}\, u$ can be evaluated by*

$$\mathcal{I}\, u = \mathcal{J}_d(2)\, u,$$

where $\mathcal{J}_d$ is defined by (14).

Corollary 11. *For $s \in (0, d)$, $R \in (0, T]$, $T \in (0, 2]$ the integral $\mathcal{J}_d(R)\, U_s$ can be estimated by*

$$\mathcal{J}_d(R)\, U_s \in \big[C_{L,d}(T), C_{H,d}\big)\, \frac{R^{d-s}}{d-s}, \tag{15}$$

where $C_{L,d}$ and $C_{H,d}$ are defined by (13).

Lemma 12. *Let X be a spherical code with cardinality $|X| = N > 2$ and minimum Euclidean distance Δ. For $x \in X$, for $R \in (\Delta, \sqrt{2}]$, the normalized counting measure σ_X of the spherical cap $S(x, R)$ can be estimated by*

$$\sigma_X\big(S(x, R)\big) := \frac{|X \cap S(x, R)|}{|X|} \leqslant 4^d \frac{C_{H,d}}{C_{L,d}(\sqrt{2})} \left(\frac{R}{\Delta}\right)^d N^{-1} = 2^{5d/2-1} \left(\frac{R}{\Delta}\right)^d N^{-1}.$$

6 Proof of Theorem 1

We fix d and drop all subscripts d where this does not cause confusion. We fix $s \in (0, d)$, fix a sequence $\mathcal{X}$ having the required properties. We also fix ℓ, drop all subscripts ℓ, and examine the spherical code $X := \{x_1, \ldots, x_N\}$. We use the abbreviations $\mathrm{E} := \mathrm{E}(X)$, $U := U_s$, $\Delta := \Delta(N)$, $\delta := \delta(N)$.

We calculate the normalized energy $\mathrm{E}\, U$ using a sum of Riemann-Stieltjes integrals, one for each of the N nodes. We have

$$\mathrm{E}\, U = \frac{1}{N} \sum_{k=1}^{N} \mathrm{E}_k\, U$$

where for any integrable function $u : (0,2] \to \mathbb{R}$,

$$\mathrm{E}_k\, u := \frac{1}{N} \sum_{\substack{j=1 \\ j \neq k}}^{N} u\left(\|x_k - x_j\|\right).$$

We use the punctured normalized counting function g_k defined by

$$g_k(r) := \sigma\big(S(x_k, r) \backslash \{x_k\}\big) = \frac{|X \cap S(x_k, r)| - 1}{N}.$$

Then

$$\mathrm{E}_k\, u = \int_0^2 u(r)\, dg_k(r) = \int_\Delta^2 u(r)\, dg_k(r).$$

where the last equation is a result of the separation condition (3). If u is differentiable on $(\Delta, 2]$ we can integrate by parts to obtain

$$\mathrm{E}_k\, u = [u(r) g_k(r)]_\Delta^2 - \int_\Delta^2 g_k(r)\, du(r) = u(2)\left(1 - N^{-1}\right) - \int_\Delta^2 D g_k(r)\, du(r).$$

Since $U(r) = r^{-s}$, we have $dU(r) = -s r^{-s-1}\, dr$, and so

$$\mathrm{E}_k\, U = 2^{-s}(1 - N^{-1}) + \int_\Delta^2 s r^{-s-1}\, g_k(r)\, dr. \tag{16}$$

Upper bound

We use the packing argument of Lemma 12 to show that

$$g_k(r) \leqslant C_1\, \Delta^{-d} N^{-1} r^d - N^{-1},$$

where

$$C_1 := 2^{5d/2-1}.$$

From the normalized spherical cap discrepancy δ and Lemma 8 we also know that

$$g_k(r) \leqslant \mathcal{V}(r) + \delta - N^{-1} \leqslant C_2\, r^d + \delta - N^{-1},$$

where

$$C_2 := \frac{C_{H,d}}{d}.$$

We now find the point ρ where these two upper bounds are equal. We want

$$C_1\, \Delta^{-d} N^{-1} \rho^d = C_2\, \rho^d + \delta,$$

so we need $(C_1\, \Delta^{-d} N^{-1} - C_2)\, \rho^d = \delta$, and we therefore define

$$\begin{aligned} \rho &:= \left(\frac{1}{C_1\, \Delta^{-d} N^{-1} - C_2}\right)^{\frac{1}{d}} \delta^{1/d} \\ &= \left(\frac{1}{C_1 - C_2\, \Delta^d N}\right)^{\frac{1}{d}} \delta^{1/d}\, \Delta N^{1/d}. \end{aligned} \tag{17}$$

We know that $\Delta^d N$ is at most $\mathrm{O}(1)$, so

$$\rho = \mathrm{O}(\delta^{1/d}\,\Delta\, N^{1/d}) \tag{18}$$

We now have

$$g_k(r) \leqslant h(r) := \begin{cases} 0, & r \in [0,\Delta] \\ C_1\,\Delta^{-d} N^{-1} r^d - N^{-1}, & r \in (\Delta,\rho) \\ \mathcal{V}(r) + \delta - N^{-1}, & r \in [\rho, 2]. \end{cases}$$

On substitution back into (16) we obtain

$$\begin{aligned} \mathrm{E}_k\, U &= 2^{-s}(1-N^{-1}) + \int_\Delta^\rho s r^{-s-1}\, g_k(r)\, dr + \int_\rho^2 s r^{-s-1}\, g_k(r)\, dr \\ &\leqslant 2^{-s}(1-N^{-1}) + C_1\,\Delta^{-d} N^{-1} \int_\Delta^\rho s r^{d-s-1}\, dr \\ &\quad + \int_\rho^2 s r^{-s-1}\, \mathcal{V}(r)\, dr + \delta \int_\rho^2 s r^{-s-1}\, dr - N^{-1} \int_\Delta^2 s r^{-s-1}\, dr \\ &= 2^{-s}(1-N^{-1}) + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\quad + \int_\rho^2 s r^{-s-1}\, \mathcal{V}(r)\, dr + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}). \end{aligned}$$

We see that this upper bound is independent of our code point index k and therefore we have

$$\begin{aligned} \mathrm{E}\, U &\leqslant 2^{-s}(1-N^{-1}) + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\quad + \int_\rho^2 s r^{-s-1}\, \mathcal{V}(r)\, dr + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}). \end{aligned}$$

Using (14), we have

$$\mathcal{I}\, U = \int_0^2 U(r)\, d\mathcal{V}(r) = U(2) - \int_0^2 DU(r)\, \mathcal{V}(r)\, dr = 2^{-s} + \int_0^2 s r^{-s-1}\, \mathcal{V}(r)\, dr.$$

Using (17) we therefore have

$$\begin{aligned} \mathrm{E}\, U - \mathcal{I}\, U &\leqslant -2^{-s} N^{-1} + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\quad - \int_0^\rho s r^{-s-1}\, \mathcal{V}(r)\, dr + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}) \\ &= -2^{-s} N^{-1} + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\quad + \rho^{-s}\,\mathcal{V}(\rho) - \int_0^\rho r^{-s}\, d\mathcal{V}(r) + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}), \end{aligned}$$

where the last equation is obtained by integration by parts.

We now use the estimate (15) to obtain

$$\begin{aligned} \mathrm{E}\, U - \mathcal{I}\, U &\leqslant -2^{-s} N^{-1} + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\quad + \rho^{-s}\,\mathcal{V}(\rho) - C_3\,\frac{1}{d-s}\rho^{d-s} + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}) \\ &\leqslant C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,\rho^{d-s} + C_2 \rho^{d-s} + \delta\,\rho^{-s} \\ &\quad - (C_1\,\frac{s}{d-s} + 1)\Delta^{-s} N^{-1} - C_3\,\frac{1}{d-s}\rho^{d-s} - 2^{-s}\,\delta\,. \end{aligned}$$

where $C_3 := C_{L,d}(\sqrt{2})$.

Substituting the order estimate $\rho = \mathrm{O}(\delta^{1/d}\,\Delta\,N^{1/d})$ from (18) we obtain

$$\mathrm{E}\,U - \mathcal{I}\,U \leqslant \mathrm{O}(\delta^{1-s/d}\,\Delta^{-s}N^{-s/d}) + \mathrm{O}(\delta^{1-s/d}\,\Delta^{d-s}N^{1-s/d}),$$

but as mentioned above, we know that $\Delta^d N$ is at most $\mathrm{O}(1)$, so we obtain our upper bound (4).

Lower bound

Using arguments similar to those for the upper bound, we obtain

$$g_k(r) \geqslant \lambda(r) := \begin{cases} 0, & r \in [0,\tau] \\ \mathcal{V}(r) - \delta - N^{-1}, & r \in [\tau, 2], \end{cases}$$

where τ is defined by $\mathcal{V}(\tau) = \delta + N^{-1}$. Thus

$$\tau = \mathrm{O}(\delta^{1/d}). \tag{19}$$

On substitution back into (16) we obtain

$$\begin{aligned} \mathrm{E}_k\,U &= 2^{-s}(1 - N^{-1}) + \int_\tau^2 s r^{-s-1}\, g_k(r)\, dr \\ &\geqslant 2^{-s}(1 - N^{-1}) + \int_\tau^2 s r^{-s-1}\, \mathcal{V}(r)\, dr - (\delta + N^{-1}) \int_\tau^2 s r^{-s-1}\, dr \\ &= 2^{-s}(1 - N^{-1}) + \int_\tau^2 s r^{-s-1}\, \mathcal{V}(r)\, dr - (\delta + N^{-1})\,(\tau^{-s} - 2^{-s}). \end{aligned}$$

We see that this lower bound is independent of our code point index k and therefore we have

$$\mathrm{E}\,U \geqslant 2^{-s}(1 - N^{-1}) + \int_\tau^2 s r^{-s-1}\, \mathcal{V}(r)\, dr - (\delta + N^{-1})\,(\tau^{-s} - 2^{-s}).$$

Similarly to the argument for the upper bound, we obtain

$$\begin{aligned} \mathcal{I}\,U - \mathrm{E}\,U &\leqslant 2^{-s}N^{-1} + \int_0^\tau s r^{-s-1}\, \mathcal{V}(r)\, dr + (\delta + N^{-1})\,(\tau^{-s} - 2^{-s}) \\ &= 2^{-s}N^{-1} - \tau^{-s}\,\mathcal{V}(\tau) + \int_0^\tau r^{-s}\, d\mathcal{V}(r) + (\delta + N^{-1})\,(\tau^{-s} - 2^{-s}) \\ &\leqslant \mathrm{O}(N^{-1}) + \mathrm{O}(\tau^{d-s}) + \mathrm{O}(\delta\ \tau^{-s}) + \mathrm{O}(N^{-1}\,\tau^{-s}). \end{aligned}$$

Using (19) we now have

$$\mathcal{I}\,U - \mathrm{E}\,U \leqslant \mathrm{O}(N^{-1}) + \mathrm{O}(\delta^{1-s/d}) + \mathrm{O}(N^{-1}\ \delta^{-s/d}),$$

yielding our lower bound (5). □

Remarks

1. The proof assumes that $\Delta < \rho < 2$. This is justified by the order estimate $\rho = \mathrm{O}(\delta^{1/d}\,\Delta\,N^{1/d})$, because $\delta(N)\,N$ is at least $\Omega(1)$, $\Delta(N)\,N^{1/d}$ is at most $\mathrm{O}(1)$, and $\delta(N) \to 0$ as $N \to \infty$.

   The proof also assumes that $\Delta < \tau < 2$. This is true for sufficiently large N, because we know that $\delta(N) = \Omega(N^{-1/2-1/2d})$ from [2], and $\delta(N) \to 0$.

2. The technique used to prove Theorem 1 might be able to be adapted for use with any smooth compact manifold, if the potential is a function of geodesic distance in the manifold itself as opposed to Euclidean distance in the embedding space, and the normalized spherical cap discrepancy is defined using balls defined via geodesic distance.

   For the proof to work properly, it would probably be necessary for the manifold to satisfy the equivalent of the standard packing argument, this time for small geodesic balls inside larger geodesic balls.

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