Discrepancy, separation and energy on spheres and on compact connected Riemannian manifolds

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Topics

- Discrepancy, separation and energy of finite sets on the unit sphere
- Examples of sequences of spherical codes whose energy converges to the continuous limit
- Generalization to compact connected Riemannian manifolds

The unit sphere, spherical codes, area measure

For $d \geqslant 2$ consider the unit sphere

$$\mathbb{S}^d := \left\{ x \in \mathbb{R}^{d+1} \mid \|x\| = 1 \right\}.$$

Let σ_d be the area measure on $\mathbb{S}^d$.

Let $\sigma := \sigma_d / \sigma_d(\mathbb{S}^d)$, so $\sigma(\mathbb{S}^d) = 1.$

Normalized spherical cap discrepancy

For any probability measure μ on $\mathbb{S}^d$, the normalized spherical cap discrepancy is

$$\mathcal{D}(\mu) := \sup_{x \in \mathbb{S}^d,\ 0<\theta<\pi} \left|\mu\big(B_x(\theta)\big) - \sigma\big(B_x(\theta)\big)\right|,$$

where $B_x(\theta)$ is the spherical cap of spherical radius θ about the point x.

(Beck and Chen 1987)

Normalized spherical cap discrepancy of a spherical code

Call a finite set of points of $\mathbb{S}^d$ a spherical code.

For a spherical code $X \subset \mathbb{S}^d$, let σ_X be the normalized counting measure defined for $Y \subset \mathbb{S}^d$ by

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

The normalized spherical cap discrepancy of X is $\mathcal{D}(X) = \mathcal{D}(\sigma_X)$.

This is the maximum 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. (Beck and Chen 1987)

Asymptotic equidistribution

A sequence $\mathcal{X} := (X_1, X_2, \ldots)$, of spherical codes is asymptotically equidistributed if $\mathcal{D}(X_\ell) < \delta(|X_\ell|)$, where δ is a positive decreasing function $\delta : \mathbb{N} \to (0, 1]$, with $\delta(N) \to 0$ as $N \to \infty$.

(Damelin and Grabner 2003)

Normalized Riesz s energy

The normalized Riesz s energy of a finite set $X \subset \mathbb{S}^d$ is $\mathbf{E}(X)\, U_s$, where $U_s(r) := r^{-s}$, the Riesz potential function, and $\mathbf{E}(X)$ is the normalized discrete energy functional

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

The corresponding normalized continuous energy functional is given by the double integral

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

(Riesz 1938, Smith 1956, Landkof 1972, Wagner 1990)

Separation of points

We are interested in spherical codes such that the minimum distance between code points is bounded below by a positive decreasing function $\Delta : \mathbb{N} \to (0, 2]$,

$$\|x - y\| > \Delta(|X_\ell|) \quad \text{for all } x, y \in X_\ell.$$

(Tammes 1930, Rankin 1955)

Well separated sequences of codes

The order of the lower bound $\Delta(N)$ for the separation of the sequence with the largest separation for each N is $\Omega(N^{-1/d})$.

Therefore, for all sequences of $\mathbb{S}^d$ codes, $\Delta(|X_\ell|) = \mathrm{O}(|X_\ell|^{-1/d})$.

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

(Tammes 1930, Rankin 1955)

Main result for $\mathbb{S}^d$

For the following result, an admissible sequence of spherical codes is a sequence $\mathcal{X}$ such that a discrepancy function δ and a separation function Δ exist, satisfying their respective bounds.

The (simplified) main result for $\mathbb{S}^d$ is then:

Theorem 1

For an admissible sequence $\mathcal{X}$ of $\mathbb{S}^d$ spherical codes, with discrepancy function δ, and separation function Δ, the normalized Riesz s energy for $0 < s < d$ is bounded by

$$\left|\left(\mathbf{E}(X_\ell) - \mathcal{I}\right) U_s\right| = \mathbf{O}\left(\delta(|X_\ell|)^{1-s/d}\, \Delta(|X_\ell|)^{-s}\, |X_\ell|^{-s/d}\right).$$

Corollary for well separated sequences

This result immediately implies the following.

Corollary 2

For a well separated admissible sequence $\mathcal{X}$ *of* $\mathbb{S}^d$ *spherical codes, with discrepancy function* δ, *the normalized Riesz* s *energy for* $0 < s < d$ *satisfies*

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

Sequences of spherical codes whose energy converges to the continuous limit

1. Minimum energy sequences.

   (Landkof 1972, Damelin and Grabner 2003, Brauchart 2005, Hardin and Saff 2005)

2. Well-separated spherical designs.

   (Grabner and Tichy 1993, Hesse and L 2008, L 2011).

   - For strength t, spherical cap discrepancy is $O(t^{-1})$.

3. Sequences of extremal fundamental systems.

   (Marzo and Ortega-Cerdà 2010).

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

   (Alexander 1972, Stolarsky 1973, Rakhmanov, Saff and Zhou 1994, Zhou 1995, Kuijlaars and Saff 1998, L 2007).

Minimum energy sequences (1)

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 of any $\mathbb{S}^d$ code with N code points. It is known that for $q \in (0, d)$, Ω_q is asymptotically equidistributed.

Brauchart (2005) gives a bound for the normalized spherical cap discrepancy of Ω_q of

$$\mathcal{D}(\Omega_{q,N}) = \mathrm{O}\left(N^{-\alpha/d}\right). \tag{1}$$

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

(Landkof 1972, Damelin and Grabner 2003, Brauchart 2005, Hardin and Saff 2005)

Minimum energy sequences (2)

For $q \in (d-2, d)$, Ω_q is also known to be well separated. Therefore, for $q \in (d-2, d)$ and $s \in (0, d)$, Corollary 2 implies that $\mathbf{E}(\Omega_{q,N})\, U_s \to \mathcal{I}\, U_s$ as $N \to \infty$.

Using Brauchart's bound (1) we obtain, for this case, the estimate

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

For general $q > 0$, the situation is more complicated, and the known results on discrepancy and separation split into a number of cases.

(Brauchart 2005, Dragnev and Saff 2007, L 2011)

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 $A_{i,j} := p_i(x_j)$.

A sequence Ξ of extremal fundamental systems with increasing degree t is known to be well separated (Reimer 1990). Marzo and Ortega-Cerdà have recently (2010) 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 $s \in (0, d)$.

(Reimer 1990, Sloan and Womersley 2004, Marzo and Ortega-Cerdà 2010)

Well separated, diameter-bounded equal area sequences

The sequence $\mathbf{EQP}(d)$ of recursive zonal equal area spherical codes, as described in the PhD thesis (L 2007) is well separated and has normalized spherical cap discrepancy $\mathcal{D}\left(\mathbf{EQP}(d, N)\right) = \mathbf{O}\left(N^{-1/d}\right)$.

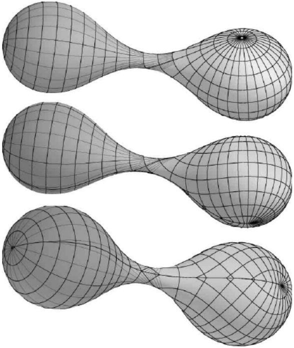
Corollary 2 therefore yields the normalized energy estimate

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

(Alexander 1972, Stolarsky 1973, Rakhmanov, Saff and Zhou 1994, Zhou 1995, Kuijlaars and Saff 1998, L 2007)

Compact connected Riemannian manifolds

Let M be a smooth, connected d-dimensional Riemannian manifold, without boundary, with metric g and geodesic distance $\mathbf{dist}$, such that M is compact in the metric topology of $\mathbf{dist}$.



(Sinclair and Tanaka, 2007, Figure 1)

Compact connected Riemannian manifolds

Let M be a smooth, connected d-dimensional Riemannian manifold, without boundary, with metric g and geodesic distance $\mathbf{dist}$, such that M is compact in the metric topology of $\mathbf{dist}$.

Let σ_M be the volume measure on M given by the volume element corresponding to g and $\mathbf{dist}$.

Since M is compact, it has finite volume.

Let $\sigma := \sigma_M/\sigma_M(M)$, so $\sigma(M) = 1$.

Normalized ball discrepancy

For any probability measure μ on M, the normalized ball discrepancy is

$$\mathcal{D}(\mu) := \sup_{x \in M,\ 0 < r < \operatorname{diam}(M)} \left| \mu\big(B_x(r)\big) - \sigma\big(B_x(r)\big) \right|,$$

where $\operatorname{diam}(M)$ is the diameter of M and $B_x(r)$ is the geodesic ball of radius r about the point x.

(Blümlinger 1990, Damelin and Grabner 2003)

Normalized Riesz s energy

The normalized Riesz s energy of an M code, a finite set $X \subset M$, is $\mathbf{E}(X)\,U_s$, where $U_s(r) := r^{-s}$, the Riesz potential function, and $\mathbf{E}(X)$ is the normalized discrete energy functional

$$\mathbf{E}(X)\,u := \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} u\,(\operatorname{dist}(x,y))\,.$$

The corresponding normalized continuous energy functional is given by the double integral

$$\mathcal{I}\,u := \int_M \int_M u\,(\operatorname{dist}(x,y))\,d\sigma(y)\,d\sigma(x).$$

(Hare and Roginskaya 2003, Damelin, et al. 2008)

Convergence of the energy of M codes

Conjecture 1

Let M be a compact connected Riemannian manifold without boundary.

For a well-separated admissible sequence $\mathcal{X}$ of M codes, the normalized Riesz s energy converges to the energy double integral of the normalized volume measure σ as $|X_\ell| \to \infty$. That is,

$$\left|\left(\mathbf{E}(X_\ell) - \mathcal{I}\right) U_s\right| \to 0 \quad \text{as } |X_\ell| \to \infty.$$

Proof (sketch)

The proof proceeds along the lines of the proof in (L 2011), except for two points.

1. The normalized potential function

$$\int_M U_s\left(\operatorname{dist}(x, y)\right) d\sigma(y)$$

varies with x, unlike the case of the sphere. This makes the conclusion of Conjecture 1 weaker.

2. The volume of a geodesic ball does not behave in exactly the same way as the volume of a spherical cap. Luckily the appropriate estimate is good enough to obtain the result.

The key estimate

Blümlinger (1990, Lemma 2) gives an estimate related to the Bishop-Gromov inequality. In our notation, it states:

Lemma 3

Let M be a compact connected d-dimensional Riemannian manifold without boundary. Then

$$\frac{\sigma_d\big(B_x(r)\big)}{\sigma_0(r)} - 1 = \mathrm{O}(r^2)$$

uniformly in M, where $\sigma_0(r)$ is the volume of the Euclidean ball of radius r in $\mathbb{R}^d$.

Therefore (roughly) the volume of a small enough geodesic ball in M is similar to the volume of a spherical cap of the same radius in $\mathbb{S}^d$. (Bishop and Crittenden 1964, Gromov 1981, Grove 1987, Echenburg 1987, Blümlinger 1990)