Discrepancy, separation and Riesz energy of finite point sets on compact connected Riemannian manifolds

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Topics

- Discrepancy, separation and energy on the unit sphere
- Generalization to compact connected Riemannian manifolds
- The main result
- A sketch of the proof
- Further questions

Result for $\mathbb{S}^d \subset \mathbb{R}^{d+1}$

In 2004, here at Vanderbilt University, Ed Saff asked me a question about, separation, discrepancy and discrete energy on the unit sphere $\mathbb{S}^d$. The answer to this question is:

Theorem 1

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 the inequality

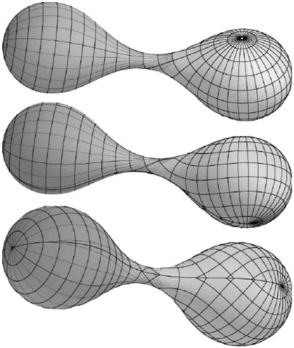
$$\mathbf{E}_{X_\ell}\, U_s = \mathbf{E}_M\, U_s + \mathbf{O}\left(\, \delta(|X_\ell|)^{1-s/d}\right).$$

This talk describes a generalization of this result.

(L 2007, L 2013)

Compact connected Riemannian manifolds

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



(Sinclair and Tanaka, 2007, Figure 1)

Metric and measure, sequences of M-codes

Let λ_M be the volume measure on M given by the volume element corresponding to g and therefore to `dist`.

Since M is compact, it has finite volume.

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

Consider an infinite sequence $\mathcal{X} := (X_1, X_2, \ldots)$ of M-codes, each a finite subset of M.

A sequence $(X_1, X_2, \ldots)$ whose cardinalities $(|X_1|, |X_2|, \ldots)$ diverge to $+\infty$ is called pre-admissible.

Normalized ball discrepancy

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

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

where $\mathtt{diam}(M)$ is the diameter of M and $B_x(r)$ is the geodesic ball of radius r about the point x.
An M-code X with cardinality $|X|$ has probability measure

$$\sigma_X(S) := |S \cap X| \, / \, |X|,$$

and therefore normalized ball discrepancy

$$\mathcal{D}(X) := \sup_{y \in M,\ r > 0} \left| |B_y(r) \cap X| \, / \, |X| - \sigma_M(B_y(r)) \right|.$$

(Blümlinger 1990, Damelin and Grabner 2003)

Asymptotic equidistribution

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

It is easy to see that $\delta(|X|) > 1/|X|$.

Consider each $B_x(r)$ with $x \in X$, and the limit as $r \to 0$.

(Blümlinger 1990, Damelin and Grabner 2003)

Separation of points, admissible sequences

An admissible sequence of M-codes is an asymptotically equidistributed pre-admissible sequence with discrepancy function δ that also has a lower bound on the minimum separation:

$$\mathtt{dist}(x, y) > \Delta(N_\ell) \quad \text{for all } x, y \in X_\ell,$$

where $\Delta : \mathbb{N} \to (0, \infty)$ is a positive decreasing function with $\Delta(N) \to 0$ as $N \to \infty$.

(Tammes 1930, Rankin 1955, Flatto and Newman 1977)

Well separated sequences of codes

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

Therefore, for all sequences of $\boldsymbol{M}$-codes,
$\boldsymbol{\Delta}(|\boldsymbol{X}_\ell|) = \mathbf{O}(|\boldsymbol{X}_\ell|^{-1/d})$.

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

(Tammes 1930, Rankin 1955, Flatto and Newman 1977)

Normalized Riesz s energy

The normalized normalized Riesz s energy of an M code is $\mathbf{E}_X\ U_s$, where $U_s(r) := r^{-s}$ and $\mathbf{E}_X$ is the normalized discrete energy functional

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

for $u : (0, \infty) \to \mathbb{R}$.

The corresponding normalized continuous energy functional is

$$\mathbf{E}_M\, u := \int_M \int_M u\left(\mathtt{dist}(x, y)\right) d\sigma_M(y)\, d\sigma_M(x).$$

(Riesz 1938, Smith 1956, Landkof 1972, Wagner 1990, Damelin et al. 2009, Hare and Roginskaya 2003)

Convergence of the energy of M codes

The generalization of the result on the unit sphere $\mathbb{S}^d$ is:

Theorem 2

Let M be a compact connected d-dimensional Riemannian manifold. If $0 < s < d$ then, for a well separated admissible sequence $\mathcal{X}$ of M-codes,

$$\left|\left(\mathbf{E}_{X_\ell} - \mathbf{E}_M\right) U\right| = \mathbf{O}\left(\delta(|X_\ell|)^{(1-s/d)/(d+2-s/d)}\right),$$

where $\delta(|X_\ell|)$ is the upper bound on the geodesic ball discrepancy of X_ℓ used to satisfy the admissibility condition.

Proof (sketch)

The proof proceeds along the lines of the proof for the sphere, except for two issues.

1. The volume of a geodesic ball does not behave in exactly the same way as the volume of a spherical cap.
2. The normalized mean potential function

$$\Phi_M(x) := \int_M U_s\left(\mathtt{dist}(x, y)\right) d\sigma_M(y)$$

varies with x, unlike the case of the sphere.

Both issues are overcome using estimates from Blümlinger (1990).

Blümlinger's first estimate

Blümlinger (1990) gives us the estimate:

Lemma 3

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

$$\left|\frac{\lambda_M(B_x(r))}{\mathcal{V}_d(r)} - 1\right| = O(r^2)$$

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

That is, the unnormalized volume of a small enough geodesic ball in M is similar to the volume of a ball of the same radius in $\mathbb{R}^d$.

(Blümlinger 1990)

Blümlinger's second estimate

Blümlinger (1990) also yields the following estimate.

Theorem 4

For $f \in C(M)$, *and a measure* ν *on* M *where* $\nu(M) = \lambda_M(M)$,

$$|\nu(f) - \lambda_M(f)| \leqslant T_1(r) + T_2(r) + T_3(r),$$

where

$$T_1(r) := \|f - f_r\|_\infty \lambda_M(M),$$

$$T_2(r) := 2\,\|f\|_\infty \lambda_M(M) \sup_{x \in M} \left| \frac{\lambda_M\big(B(x,r)\big)}{\mathcal{V}_d(r)} - 1 \right|,$$

$$T_3(r) := \frac{\|f\|_\infty}{\mathcal{V}_d(r)} \int_M \left|\nu\big(B(x,r)\big) - \lambda_M\big(B(x,r)\big)\right|\, d\,\lambda_M(x).$$

Some notation

For integrable $f : M \to \mathbb{R}$, the mean of f on M is

$$\mathcal{I}_M f := \int_M f(y)\, d\sigma_M(y).$$

For a function $f : M \to \mathbb{R}$ that is finite on the M-code X, the mean of f on X is

$$\mathcal{I}_X f := \int_M f(y)\, d\sigma_X(y) = \frac{1}{|X|} \sum_{y \in X} f(y).$$

Some notation

For an M-code X, a point $x \in M$ and a measurable subset $S \subset M$, the punctured normalized counting measure of S with respect to X, excluding x is

$$\sigma_X^{[x]}(S) := |S \cap X \setminus \{x\}| \,/\, |X|,$$

and for a function $f : M \to \mathbb{R}$ that is finite on $X \setminus \{x\}$, the corresponding punctured mean is

$$\mathcal{I}_X^{[x]} f := \int_M f(y)\, d\sigma_X^{[x]}(y) = \frac{1}{|X|} \sum_{\substack{y \in X \\ y \neq x}} f(y).$$

Some notation

For a point $x \in M$, define the function $U_x : M \setminus \{x\} \to \mathbb{R}$ as

$$U_x(y) := \mathtt{dist}(x, y)^{-s}.$$

The mean Riesz s-potential at x with respect to M is then

$$\Phi_M(x) = \mathcal{I}_M U_x,$$

and the normalized energy of the Riesz s-potential on M is

$$\mathbf{E}_M\, U = \mathcal{I}_M \Phi_M = \int_M \int_M \mathtt{dist}(x, y)^{-s}\, d\sigma_M(y)\, d\sigma_M(x).$$

Some notation

For an M-code X, the mean Riesz s-potential at x with respect to X but excluding x is

$$\Phi_X(x) := \mathcal{I}_X^{[x]} U_x,$$

the normalized energy of the Riesz s-potential on X is

$$\mathbf{E}_X\, U = \mathcal{I}_X \Phi_X = \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} \mathtt{dist}(x, y)^{-s},$$

and the mean on X of the mean Riesz s-potential is

$$\mathcal{I}_X \Phi_M = \frac{1}{|X|} \sum_{x \in X} \int_M \mathtt{dist}(x, y)^{-s}\, d\sigma_M(y).$$

Proof (sketch, continued)

First, split the energy difference $\left(\mathbf{E}_X - \mathbf{E}_M\right) U$ into two parts:

$$\begin{aligned}\left(\mathbf{E}_X - \mathbf{E}_M\right) U &= \mathcal{I}_X \Phi_X - \mathcal{I}_M \Phi_M \\ &= (\mathcal{I}_X \Phi_X - \mathcal{I}_X \Phi_M) + (\mathcal{I}_X \Phi_M - \mathcal{I}_M \Phi_M) \\ &= \mathcal{I}_X (\Phi_X - \Phi_M) + (\mathcal{I}_X - \mathcal{I}_M) \Phi_M.\end{aligned}$$

Next, estimate each part.

Lemma 3 yields the estimate

$$|\mathcal{I}_X (\Phi_X - \Phi_M)| = \mathrm{O}(\delta^{1-s/d}).$$

Proof (sketch, continued)

We apply Theorem 4 with $f := \Phi_M$ and $\nu := \lambda(M)\sigma_X$.

It turns out that for r sufficiently small,

$$T_1(r) = \mathrm{O}(r^{(d-s)/(d+1)}).$$

Lemma 3 yields $T_2(r) = \mathrm{O}(r^2)$.
The bound $\big|\nu\big(B(x,r)\big) - \lambda_M(B(x,r))\big| \leqslant \delta\,\lambda(M)$ yields

$$T_3(r) = \mathrm{O}(\delta\, r^{-d}).$$

Setting $r = \delta^{(d+1)/(d^2+2d-s)}$ then results in the estimate

$$|(\mathcal{I}_X - \mathcal{I}_M)\Phi_M| = \mathrm{O}\left(\delta^{(d-s)/(d^2+2d-s)}\right).$$

Questions

1. Is the convergence rate given in Theorem 2 best possible?
2. For a compact connected Riemannian manifold M, for what function spaces F_M does a Koksma-Hlawka type inequality

$$|(\mathcal{I}_X - \mathcal{I}_M)f| \leqslant \mathcal{D}(X)\; V(f)$$

hold for all $f \in F_M$, where $\mathcal{D}(X)$ is the geodesic ball discrepancy? What is the appropriate functional V?
3. For which compact connected Riemannian manifolds M does the space F_M contain the mean potential function Φ_M?
4. For which compact connected Riemannian manifolds M is there an efficient construction for a well-separated admissible sequence $\mathcal{X}$?