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

Paul Leopardi

Mathematical Sciences Institute, Australian National University.

For presentation at Optimal Point Configurations and Applications 2014, ESI Vienna

14 October 2014

Acknowledgements

Vanderbilt University Ed Saff and Doug Hardin.

UNSW Johann Brauchart, Kerstin Hesse, Ian Sloan and Rob Womersley.

TU Wien Martin Blümlinger.

U Padova Stefano De Marchi, Alvise Sommariva and Marco Vianello.

U Milano Leonardo Colzani.

U Bergamo Giacomo Gigante.

ANU Lashi Bandara, Julie Clutterbuck, Thierry Coulhon, Mat Langford and David Shellard.

DRNA Ronald Cools and Anonymous Referee.

Erwin Schrödinger Institute, Australian Research Council.

Pozible supporters

$32+ SvA, AD, CF, OF, KM, JP, AHR, RR, ES, MT.

$50+ Yvonne Barrett, Angela M. Fearon, Sally Greenaway, Dennis Pritchard, Susan Shaw, Bronny Wright.

$64+ Naomi Cole.

$100+ Russell family, Jonno Zilber.

$128+ Jennifer Lanspeary, Vikram.

. . . and others, who did not want acknowledgement.

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

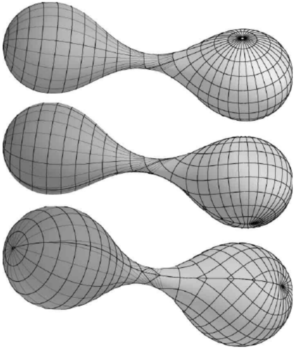
$$\mathbf{E}_{X_\ell}\, U_s = \mathbf{E}_M\, U_s + \mathbf{O}\left(\, \delta(|X_\ell|)^{1-s/d}\right).$$

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

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

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

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

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

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

A sequence of M-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, 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

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

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

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

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

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

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 $\left|\nu\big(B(x,r)\big) - \lambda_M\big(B(x,r)\big)\right| \leqslant \delta\,\lambda(M)$ 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 $\mathcal{X}$?