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

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Abstract For the unit sphere $\mathbb{S}^d \in \mathbb{R}^{d+1}$, if $0 < s < d$ then an asymptotically equidistributed sequence of spherical codes that is also well-separated yields a sequence of Riesz s-energies that converges to the energy double integral, with the rate of convergence depending on the spherical cap discrepancy [17]. In the more general case of a smooth compact connected d-dimensional Riemannian manifold, where the corresponding discrepancy is based on geodesic balls, the Riesz s-energy also converges to the energy double integral, but the rate of convergence is not yet known.

Keywords compact Riemannian manifold · ball discrepancy · equidistribution · separation · Riesz energy

Mathematics Subject Classification (2000) 11K38 · 41A55 · 65D30

1 Introduction and Main Results

For $d \geqslant 2$ let M be a smooth connected d-dimensional Riemannian manifold, without boundary, with metric g and geodesic distance $\mathtt{dist}$, such that M is compact in the metric topology of $\mathtt{dist}$. Let $\mathtt{diam}(M)$ be the *diameter* of M, the maximum geodesic distance between points of M. Let λ_M be the volume measure on M given by the volume element corresponding to g. Since M is compact, it has finite diameter and finite volume. Let σ_M be the probability measure $\lambda_M/\lambda_M(M)$ on M. For the remainder of this paper, all compact connected Riemannian manifolds are assumed to be finite dimensional, smooth and without boundary.

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

$$\mathscr{D}(\mu) := \sup_{x \in M,\ r>0} \left|\mu\big(B(x,r)\big) - \sigma\big(B(x,r)\big)\right|,$$

where $B(x,r)$ is the geodesic ball of radius r about the point x [2,7].

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This paper concerns infinite sequences $\mathscr{X} := (X_1, X_2, \ldots)$ of finite subsets of the manifold M. Each such finite subset is called an *M-code*, by analogy with spherical codes, which are finite subsets of the unit sphere $\mathbb{S}^d$. A sequence $(X_1, X_2, \ldots)$ whose corresponding sequence of cardinalities $(|X_1|, |X_2|, \ldots)$ diverges to $+\infty$ is called a *preadmissible* sequence of M-codes.

An M-code X with cardinality $|X|$ has a corresponding probability measure σ_X and normalized ball discrepancy $\mathscr{D}(X)$, where for any measurable subset $S \subset M$,

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

and

$$\mathscr{D}(X) := \mathscr{D}(\sigma_X) = \sup_{y \in M,\ r>0} \left| |B(y,r) \cap X| \,/\, |X| - \sigma\big(B(y,r)\big) \right|.$$

It is easy to see $\mathscr{D}(X) \geqslant 1/|X|$, since for any $x \in X$, $\sigma\big(B(x,\varepsilon)\big)$ can be made arbitrarily small by taking $\varepsilon \to 0$, while $\sigma_X\big(B(x,\varepsilon)\big)$ must always remain at least $1/|X|$.

A preadmissible sequence $\mathscr{X} := (X_1, X_2, \ldots)$, of M-codes with corresponding cardinalities $N_\ell := |X_\ell|$ is *asymptotically equidistributed* [7, Remark 4, p. 236], if the normalized ball discrepancy is bounded above as per

$$\mathscr{D}(X_\ell) < \delta(N_\ell), \tag{1}$$

where $\delta : \mathbb{N} \to (0,1]$, is a positive decreasing function with $\delta(N) \to 0$ as $N \to \infty$.

The preadmissible sequences of M-codes of most interest for this paper are those such that the minimum geodesic distance between code points is bounded below by a positive decreasing function $\Delta : \mathbb{N} \to (0,\infty)$,

$$\mathtt{dist}(x,y) > \Delta(N_\ell) \quad \text{for all } x, y \in X_\ell. \tag{2}$$

An easy area argument shows that the order of the lower bound $\Delta(N)$ for the sequence of M-codes having the largest minimum geodesic distance for each N is $\Omega(N^{-1/d})$. (See also Flatto and Newman [11, Theorem 2.2].) Therefore, for all sequences of M-codes,

$$\Delta(N_\ell) = \mathrm{O}(N_\ell^{-1/d}), \tag{3}$$

where the implied constant depends on M and therefore on d, but does not depend on N. A sequence of M-codes is called *well separated* if there exists a *separation constant* $\gamma > 0$ such that we can set $\Delta(N) = \gamma N^{-1/d}$.

For the purposes of this paper, we define an *admissible sequence* of M-codes to be a preadmissible sequence $\mathscr{X}$, such that a discrepancy function δ, and a separation function Δ exist, satisfying the bounds (1) and (2) respectively.

The normalized *normalized Riesz s-energy* of an M-code is $\mathrm{E}_X\, U^{(s)}$, where E_X is the normalized discrete energy functional

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

and $U^{(s)}(r) := r^{-s}$, the Riesz potential function.

The corresponding normalized continuous energy functional is given by the double integral [9, 14]

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

The main result of this paper is the following theorem.

Theorem 1.1 *Let M be a compact connected d-dimensional Riemannian manifold. If $0 < s < d$ then, for a well separated admissible sequence $\mathscr{X}$ of M-codes, the normalized Riesz s-energy converges to the energy double integral of the normalized volume measure σ_M as $|X_\ell| \to \infty$. That is,*

$$\left|\left(\mathrm{E}_{X_\ell} - \mathrm{E}_M\right) U^{(s)}\right| \to 0 \quad \textit{as } |X_\ell| \to \infty.$$

The proof of Theorem 1.1 is given in Section 3 below. This proof is similar to that of Theorem 1.1 in the corresponding paper on the unit sphere [17], except for two key points of difference:

1. The *normalized mean potential function*

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

may vary with x, unlike the case of the sphere, where the corresponding mean potential function is a constant.
2. The volume of a geodesic ball in general 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.

Blümlinger [2, Lemma 2] gives an estimate related to the *Bishop-Gromov inequality* [1, 11.10, pp. 253–257] [12, Lemma 5.3bis pp. 65–66] [13, Lemma 5.3bis pp. 275–277]. In the notation used here, Blümlinger's estimate states:

Let M be a compact connected d-dimensional Riemannian manifold. Then

$$\frac{\lambda_M\left(B(x,r)\right)}{\mathscr{V}_d(r)} - 1 = \mathrm{O}(r^2) \tag{4}$$

uniformly in M, where $\mathscr{V}_d(r)$ 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 $\mathbb{R}^d$, to the order of the square of the radius. (See also Flatto and Newman [11, Theorem 2.3 and Remarks].)

The proof of Lemma 2 in Blümlinger's paper [2] makes it clear that the order estimate is valid for $r < R_0$, where R_0 is the *injectivity radius* of M [1, Lemma 3, Section 8.2, p. 153] [18, Definition 4.12, p. 110]. Thus, Blümlinger's estimate can be restated as the following result.

Lemma 1.2 *Let M be a compact connected d-dimensional Riemannian manifold, and let R_0 be the injectivity radius of M. There exists a real positive constant C_0 such that for $r \in (0, R_{0,m})$*

$$\left| \frac{\lambda_M\big(B(x,r)\big)}{\mathscr{V}_d(r)} - 1 \right| \leqslant C_0 r^2 \tag{5}$$

uniformly in M.

2 Notation and results used in the proof of Theorem 1.1

The proof of Theorem 1.1 needs some notation and a few results, which are stated here. The first two results follow from Blümlinger's estimate.

Lemma 2.1 *Let M be a compact connected d-dimensional Riemannian manifold. There is a radius $R_1 > 0$ and parameters $0 < C_L < C_H$, depending on R_1, such that for all $x \in M$ and all $r \in (0, R_1)$,*

$$C_L\, r^d \leqslant \sigma_M\,(B(x,r)) \leqslant C_H\, r^d. \tag{6}$$

The ratio C_H/C_L can be made arbitrarily close to 1 by taking R_1 arbitrarily close to 0.

Proof Let $R_0 > 0$ be the injectivity radius of M, so that Blümlinger's estimate (5) holds for $r \in (0, R_0)$. Note that for each d, $\mathscr{V}_d(r) = c_d r^d$, where $c_d := \mathscr{V}_d(1) > 0$. It follows that for all $r \in (0, R_0)$ the estimate

$$c_d r^d (1 - C_0 r^2) \leqslant \lambda_M\big(B(x,r)\big) \leqslant c_d r^d (1 + C_0 r^2) \tag{7}$$

holds for some $C_0 > 0$. Let $R_1 \in (0, R_0)$ satisfy $C_0 R_1^2 < 1$ so that the lower bound in the estimate (7) is positive for $r \in (0, R_1)$. It follows that for all $r \in (0, R_1)$,

$$0 < \frac{c_d(1 - C_0 R_1^2)}{\lambda_M(M)} r^d \leqslant \lambda_M\big(B(x,r)\big) \leqslant \frac{c_d(1 + C_0 R_1^2)}{\lambda_M(M)} r^d.$$

The estimate (6) therefore holds for R_1 as above, $C_L := c_d(1 - C_0 R_1^2)/\lambda_M(M)$, and $C_H := c_d(1 + C_0 R_1^2)/\lambda_M(M)$. In this case,

$$\frac{C_H}{C_L} = \frac{1 + C_0 R_1^2}{1 - C_0 R_1^2} \quad \to 1, \quad \text{as} \quad R_1 \to 0. \qquad \square$$

Lemma 2.2 *Let M be a compact connected d-dimensional Riemannian manifold. For $x \in M$ and real $r > t > 0$ let $n_M(x,r,t)$ be the maximum number of geodesic balls of radius t that can be contained in the ball $B(x,r)$. Then there is a radius R_2 and a constant C_2 such that for all $x \in M$, $r \in (0, R_2)$, and $q \in (0, r)$,*

$$n_M(x, r + q/2, q/2) \leqslant C_2\,(r/q)^d. \tag{8}$$

In other words, for small enough real positive r, for $0 < q < r$, the maximum number of geodesic balls of radius $q/2$ that can be contained in a geodesic ball of radius $r + q/2$ is of order $\mathrm{O}(r/q)^d$, uniformly in M.

Proof The total volume of the small balls cannot be greater than the volume of the large ball containing them. Using Lemma 2.1, it therefore holds for $0 < q < r \leqslant 2R_1/3$ that

$$\begin{aligned} n_m(x, r+q/2, q/2) &\leqslant \frac{\max_{y\in M} \sigma_M\big(B(y, r+q/2)\big)}{\min_{z\in M} \sigma_M\big(B(z, q/2)\big)} \\ &\leqslant 2^d \frac{C_H}{C_L} \left(1 + \frac{q}{2r}\right)^d (r/q)^d \leqslant 3^d \frac{C_H}{C_L} (r/q)^d. \end{aligned}$$

Thus (8) holds with $R_2 := 2R_1/3$ and $C_2 := 3^d C_H/C_L$. □

The remaining lemmas in this Section as well as the proof of Theorem 1.1 make use of the following definitions.

For $x \in M$, real radius $r > 0$, and integrable $f : B(x,r) \to \mathbb{R}$, the *normalized integral of f on the geodesic ball $B(x,r)$* is

$$\mathscr{I}_{B(x,r)} f := \int_{B(x,r)} f(y)\, d\sigma_M(y).$$

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

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

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

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

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

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

Note the division by $|X|$ rather than $|X| - 1$.

The kernel $U^{(s)}\big(\mathtt{dist}(x,y)\big) = \mathtt{dist}(x,y)^{-s}$ is called the *Riesz s-kernel.* For a point $x \in M$, define the function $U_x^{(s)} : M \setminus \{x\} \to \mathbb{R}$ as

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

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

$$\Phi_M^{(s)}(x) = \mathscr{I}_M U_x^{(s)}, \tag{9}$$

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

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

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

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

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

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

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

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

The following bound is used in the proof of Theorem 1.1.

Lemma 2.3 *Let M be a compact connected d-dimensional Riemannian manifold. Then for the radius R_1 as per Lemma 2.1, there is a constant C_3 such that for all $x \in M$ and $r \in (0, R_1)$, the normalized integral of the function $U_x^{(s)}$ is bounded as*

$$\mathscr{I}_{B(x,r)} U_x^{(s)} \leqslant C_3 r^{d-s}. \tag{10}$$

Proof Fix $x \in M$, and let $\mathscr{V}_M(r) := \sigma_M\big(B(x,r)\big)$. Then for $r \in (0, R_1)$, the following equations and inequality hold,

$$\begin{aligned}
\mathscr{I}_{B(x,r)} U_x^{(s)} &= \int_{B(x,r)} \mathtt{dist}(x,y)^{-s}\, d\sigma_M(y) = \int_0^r t^{-s}\, d\mathscr{V}_M(t) \\
&= r^{-s} \mathscr{V}_M(r) + s \int_0^r t^{-s-1} \mathscr{V}_M(t)\, dt \\
&\leqslant C_1 r^{d-s} + s \int_0^r C_1 t^{d-s-1}\, dt = C_1 \frac{d}{d-s}\, r^{d-s},
\end{aligned}$$

where the inequality is a result of Blümlinger's estimate. Thus the estimate (10) is satisfied for $C_3 = C_1\, d/(d-s)$. $\square$

The proof of Theorem 1.1 uses the continuity of the mean Riesz s-potential, as shown by the following lemma.

Lemma 2.4 *Let M be a compact connected d-dimensional Riemannian manifold. Then for $s \in (0,d)$, the mean Riesz s-potential $\Phi_M^{(s)}$ defined by* (9) *is continuous on M.*

Proof We show that the mean Riesz s-potential $\varPhi_M^{(s)}$ is continuous by using the method of proof of Kellogg [15, p. 150-151].

Let $x \in M$ and recall that $\varPhi_M^{(s)}(x) = \mathscr{I}_M U_x^{(s)}$. Let x' be another point of M and consider the ball $B'_r := B(x', r)$, for some $r \in (0, R_1/3)$ where R_1 is a suitable radius as per Lemma 2.1. Consider $\varPhi_{B'_r}^{(s)}(x) := \mathscr{I}_{B'_r} U_x^{(s)}$. Either $\mathtt{dist}(x,x') \leqslant 2r$, in which case $x' \in B(x, 2r)$ so that

$$\mathscr{I}_{B'_r} U_x^{(s)} < \mathscr{I}_{B(x,3r)} U_x^{(s)} \leqslant 3^{d-s}\, C_3\, r^{d-s}$$

as per Lemma 2.3, or $\mathtt{dist}(x,x') > 2r$, so that

$$\mathscr{I}_{B'_r} U_x^{(s)} \leqslant (2r)^{-s}\, C_H r^d = 2^{-s}\, C_H r^{d-s},$$

as per Lemma 2.1. Therefore $\varPhi_{B'_r}^{(s)} \to 0$ uniformly on M as $r \to 0$.

So, given $\varepsilon > 0$ we can take r small enough that $\varPhi_{B'_r}^{(s)}(x) < \varepsilon/2$ for all $x \in M$, and therefore $\varPhi_{B'_r}^{(s)}(x') < \varepsilon/2$, so

$$\left| \mathscr{I}_{B'_r} \left(U_x^{(s)} - U_x'^{(s)} \right) \right| < \varepsilon/2.$$

With B'_r fixed, there is a distance $t > 0$ such that when $\mathtt{dist}(x,x') \leqslant t$, we have

$$\left| U_x^{(s)}(y) - U_x'^{(s)}(y) \right| = \left| \mathtt{dist}(x,y)^{-s} - \mathtt{dist}(x',y)^{-s} \right| \leqslant \varepsilon/2$$

for all $y \in M \setminus B'_r$. In this case

$$\left| \mathscr{I}_{M\setminus B'_r} \left(U_x^{(s)} - U_x'^{(s)} \right) \right| \leqslant \mathscr{I}_{M\setminus B'_r} \left| U_x^{(s)} - U_x'^{(s)} \right| < \varepsilon/2.$$

Therefore $\left| \mathscr{I}_M \left(U_x^{(s)} - U_x'^{(s)} \right) \right| \leqslant \varepsilon$ whenever $\mathtt{dist}(x,x') \leqslant t$. $\square$

3 Proof of Theorem 1.1

Fix the manifold M and therefore fix d. Fix $s \in (0,d)$, and drop all superscripts (s) from the notation, where this does not cause confusion. Fix a sequence $\mathscr{X}$ having the required properties. Fix ℓ, drop all subscripts ℓ, and examine the spherical code $X := \{x_1, \ldots, x_N\}$, so that $|X| = N$. The notation of the proof also uses the abbreviations $\varDelta := \varDelta(N)$, $\delta := \delta(N)$.

The first observation is that

$$\begin{aligned}
\left(\mathrm{E}_{X_\ell} - \mathrm{E}_M\right) U &= \mathscr{I}_X \Phi_X - \mathscr{I}_M \Phi_M \\
&= (\mathscr{I}_X \Phi_X - \mathscr{I}_X \Phi_M) + (\mathscr{I}_X \Phi_M - \mathscr{I}_M \Phi_M) \\
&= \mathscr{I}_X (\Phi_X - \Phi_M) + (\mathscr{I}_X - \mathscr{I}_M) \Phi_M.
\end{aligned}$$

Since $\varPhi_M$ is continuous on M as per Lemma 2.4, and since the sequence $\mathscr{X}$ is asymptotically equidistributed, the term $(\mathscr{I}_X - \mathscr{I}_M)\varPhi_M$ converges to 0 as $N \to \infty$.

The remainder of the proof concentrates on the convergence to 0 of the term $\mathscr{I}_X(\Phi_X - \Phi_M)$. Since

$$\mathscr{I}_X(\Phi_X - \Phi_M) = \frac{1}{N} \sum x \in X (\Phi_X(x) - \Phi_M(x)) \tag{11}$$

the proof proceeds by placing a uniform bound on the net mean potential $\Phi_X(x) - \Phi_M(x)$ at $x \in X$. We express this net mean potential as a difference between Riemann-Stieltjes integrals, then integrate by parts.

Fix $x \in X$. The volume of the ball $B(x,r)$ with respect to the punctured normalized counting measure $\sigma_X^{[x]}$ is

$$\mathscr{V}_X^{[x]} := \sigma_X^{[x]}(B(x,r)) = \frac{|B(x,r) \cap X| - 1}{N}.$$

Using $\mathscr{V}_M(r) := \sigma_M\big(B(x,r)\big)$ to denote the volume of $B(x,r)$ with respect to the measure σ_M, and integrating by parts, yields

$$\begin{aligned}
\Phi_X(x) - \Phi_M(x) &= \mathscr{I}_X^{[x]} U_x - \mathscr{I}_M U_x \\
&= \int_M U(\mathtt{dist}(x,y))\, d\sigma_X^{[x]}(y) - \int_M U(\mathtt{dist}(x,y))\, d\sigma_M(y). \\
&= \int_0^\infty r^{-s}\, d\mathscr{V}_X^{[x]}(r) - \int_0^\infty r^{-s}\, d\mathscr{V}_M(r) \\
&= \int_0^\infty s r^{-s-1}\, \mathscr{V}_X^{[x]}(r)\, dr - \int_0^\infty s r^{-s-1}\, \mathscr{V}_M(r)\, dr \\
&= \int_0^\infty s r^{-s-1} \big(\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r)\big)\, dr.
\end{aligned} \tag{12}$$

The next step consists of bounding $\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r)$ above and below. Each of $\mathscr{V}_X^{[x]}(r)$ and $\mathscr{V}_M(r)$ have a number of bounds that apply for different values of r.

For $\mathscr{V}_M(r)$, since σ_M is a probability measure on M, $\mathscr{V}_M(r) = 1$ when $r \geqslant \mathtt{diam}(M)$. For $r < R_1$, the bounds given by Lemma 2.1 apply.

For $\mathscr{V}_X^{[x]}(r)$, since σ_X is also a probability on M, $\mathscr{V}_X^{[x]}(r) = (N-1)/N$ when $r \geqslant \mathtt{diam}(M)$. and since the minimum distance between points of X is bounded below by Δ, $\mathscr{V}_X^{[x]}(r) = 0$ when $r < \Delta$. For $r \in \big[\Delta, \mathtt{diam}(M)\big)$, the properties of X yield bounds on $\mathscr{V}_X^{[x]}(r)$.

Upper bound

Because the minimum distance between points of X is bounded below by Δ, each point of X can be placed in a ball of radius $\Delta/2$, with no two balls overlapping. Lemma 2.2 then implies that for $r < R_2$,

$$|B(x,r) \cap X| = n_M(x, r + \Delta/2, \Delta/2) \leqslant C_2\,(r/\Delta)^d,$$

and so

$$\mathscr{V}_X^{[x]}(r) \leqslant C_2\,\Delta^{-d} N^{-1} r^d - N^{-1}. \tag{13}$$

Since the normalized spherical cap discrepancy $\mathscr{D}(X)$ is bounded above by δ, it is also true that for $0 < r < \mathtt{diam}(X)$,

$$-\delta \leqslant \mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r) + N^{-1} \leqslant \delta,$$

and, for $0 < r < R_1$, as a result of Lemma 2.1,

$$\mathscr{V}_X^{[x]}(r) \leqslant C_H\, r^d + \delta - N^{-1}. \tag{14}$$

Let ρ denote the geodesic radius where the two upper bounds (13) and (14) are equal. Thus ρ is the solution of the equation

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

This is given by

$$\rho = \left(\frac{1}{C_2 - C_H\,\Delta^d N} \right)^{1/d} \delta^{1/d}\,\Delta N^{1/d}. \tag{15}$$

It follows from Lemma 2.1 and the proof of Lemma 2.2 that $C_2 \geqslant 3^d$. From Lemma 2.1 it also follows that

$$C_L\,\Delta^d \leqslant 2^d \sigma\big(B(x,\Delta/2)\big)$$

for all $x \in X$, and so

$$C_L\,\Delta^d N \leqslant 2^d \sum_{x\in X} \sigma_M\big(B(x,\Delta/2)\big) \leqslant 2^d \sigma_M(M) = 2^d,$$

since the N balls of radius $\Delta/2$ do not overlap. By making R_1 small enough, C_H/C_L can be made arbitrarily close to 1, and then $C_2 - C_H\,\Delta^d N$ is positive. Since $C_2 - C_H\,\Delta^d N < C_2$ and since $\Delta^d N = \mathrm{O}(1)$, this results in the order estimate

$$\rho = \Theta\big(\,\delta^{1/d}\big). \tag{16}$$

Therefore since $\delta \to 0$, this implies that $\rho \to 0$. Thus it is possible to set R_1 small enough that the estimates used in (15) are valid for large enough N. Also, $\delta\,N$ is at least $\Omega(1)$. Therefore $0 < \Delta < \rho < R_1$, for N sufficiently large.

The upper bounds for $\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r)$ therefore split into the cases

$$\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r) \leqslant \begin{cases} -C_L r^d, & r \in [0,\Delta], \\ (C_2\,\Delta^{-d} N^{-1} - C_L) r^d - N^{-1}, & r \in (\Delta,\rho), \\ \delta - N^{-1}, & r \in [\rho, \mathtt{diam}(M)), \\ -N^{-1}, & r \geqslant \mathtt{diam}(M). \end{cases}$$

Substitution back into (12) results in the upper bound

$$\begin{aligned}
\Phi_X(x) - \Phi_M(x) &= \int_0^\infty s r^{-s-1} \left(\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r)\right) dr \\
&\leqslant -C_L\, s \int_0^\Delta r^{d-s-1}\, dr \;+\; (C_2\, \Delta^{-d} N^{-1} - C_L)\, s \int_\Delta^\rho r^{d-s-1}\, dr \\
&\quad + \delta \int_\rho^{\mathtt{diam}(M)} s r^{-s-1}\, dr \;-\; N^{-1} \int_\Delta^\infty s r^{-s-1}\, dr \\
&= -C_L \frac{s}{d-s} \Delta^{d-s} + \left(C_2\, \Delta^{-d} N^{-1} - C_L\right) \frac{s}{d-s} \left(\rho^{d-s} - \Delta^{d-s}\right) \\
&\quad + \delta \left(\rho^{-s} - \mathtt{diam}(M)^{-s}\right) - N^{-1} \Delta^{-s}.
\end{aligned}$$

Substituting the order estimate for ρ from (16) and noting that $\Delta^d N = \mathrm{O}(1)$ and $\delta\, N$ is at least $\Omega(1)$, results in the upper bound

$$\Phi_X(x) - \Phi_M(x) \leqslant \mathrm{O}(\Delta^{d-s}) + \mathrm{O}(\delta^{1-s/d}) = \mathrm{O}(\delta^{1-s/d}). \tag{17}$$

Lower bound

Define the radius τ by $C_L \tau^d = \delta + N^{-1}$. Since $\delta \geqslant N^{-1}$ and since $\delta\, N$ is at least $\Omega(1)$,

$$\tau = \Theta\left(\delta^{1/d}\right). \tag{18}$$

Since $\Delta = \mathrm{O}(N^{-1/d})$ and since $\delta \to 0$, we must therefore have

$$0 < \Delta < \tau < \mathtt{diam}(M),$$

for N sufficiently large.

Using arguments similar to those for the upper bound results in the cases

$$\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r) \geqslant \begin{cases} -C_H r^d, & r \in [0, \tau], \\ -\delta - N^{-1}, & r \in (\tau, \mathtt{diam}(M)), \\ -N^{-1}, & r \geqslant \mathtt{diam}(M). \end{cases}$$

This lower bound is independent of the code point x. Substitution back into (12) results in the lower bound

$$\begin{aligned}
\Phi_X(x) - \Phi_M(x) &= \int_0^\infty s r^{-s-1} \left(\mathscr{V}_X^{[x]}(r) - \mathscr{V}_M(r)\right) dr \\
&\geqslant -C_H\, s \int_0^\tau r^{d-s-1}\, dr + \delta \int_\tau^{\mathtt{diam}(M)} s r^{-s-1}\, dr - N^{-1} \int_\tau^\infty s r^{-s-1}\, dr \\
&= -C_H \frac{s}{d-s} \tau^{d-s} + \delta \left(\tau^{-s} - \mathtt{diam}(M)^{-s}\right) - N^{-1} \tau^{-s}.
\end{aligned}$$

Similarly to the argument for the upper bound, and using (18), this results in the lower bound

$$\Phi_X(x) - \Phi_M(x) \geqslant -\left(\mathrm{O}(\tau^{d-s}) + \mathrm{O}(N^{-1}\tau^{-s})\right) = -\left(\mathrm{O}(\delta^{1-s/d})\right). \tag{19}$$

Final result

When the upper bound (17) is combined with the lower bound (19), this results in the overall order estimate

$$|\Phi_X(x) - \Phi_M(x)| \leqslant \mathrm{O}(\delta^{1-s/d}).$$

Therefore, recalling the sum 11, this shows that $\mathscr{I}_X(\Phi_X - \Phi_M)$ converges to 0 as $N \to \infty$. Since it has already been established that $(\mathscr{I}_X - \mathscr{I}_M)\Phi_M$ converges to 0 as $N \to \infty$, this proves Theorem 1.1. □

4 Discussion

Theorem 1.1 demonstrates the convergence of the normalized Riesz s-energy of a well separated, equidistributed sequence of M-codes on a compact connected d-dimensional Riemannian manifold M to the energy given by the double integral of the normalized volume measure on M, if $0 < s < d$, but it does not give an estimate of the rate of convergence. If the manifold M had a Koksma-Hlawka-type inequality for the ball discrepancy δ with a function space F_M containing the function Φ_M, the estimate

$$(\mathscr{I}_X - \mathscr{I}_M)\Phi_M \leqslant \delta \ V\left(\Phi_M\right)$$

would hold for some appropriate functional V on the space F_M. Unfortunately, not much is known about Koksma-Hlawka type inequalities for geodesic balls on compact connected Riemannian manifolds, with the exception of the sphere $\mathbb{S}^d$ [5, Section 3.2, p. 490] [6, Proposition 20]. The papers by Brandolini et al. [3,4] examine Koskma-Hlawka type inequalities on compact Riemannian manifolds. The main results of these two papers concern discrepancies which are not in general the same as the geodesic ball discrepancy, but they do suggest directions for further research.

Further research could address the following questions.

1. For a compact connected Riemannian manifold M, without boundary, for what linear spaces F_M does a Koksma-Hlawka type inequality
$$(\mathscr{I}_X - \mathscr{I}_M)f \leqslant \mathscr{D}(X)\, V(f) \tag{20}$$
hold, where the relevant discrepancy in the inequality is the geodesic ball discrepancy?
2. What is the appropriate functional V in (20)? Is V a norm or a semi-norm on the function space F_M?
3. For which compact connected Riemannian manifolds M does the Koksma-Hlawka function space F_M contain the mean potential function Φ_M?
4. Is there another approach to bounding the rate of convergence of the term $(\mathscr{I}_X - \mathscr{I}_M)\Phi_M$ that does not involve generalizations of the Koksma-Hlawka inequality?

Finally, no mention has yet been made of constructions for, or even the existence of, well separated, admissible sequences on compact connected Riemannian manifolds.

The case of the unit sphere $\mathbb{S}^d$ has been well studied [17] and a number of constructions are known, including one that uses a partition of the sphere into regions of equal volume and bounded diameter [16].

Damelin et al. have studied the discrepancy and energy of finite sets contained within measurable subsets of Hausdorff dimension d embedded in a higher dimensional Euclidean space, where the energy and discrepancy are both defined via an admissible kernel [8]. One of their key results is to express the discrepancy of a finite set with respect to an equilibrium measure as the square root of the difference between the energy of the finite set and the energy of the equilibrium measure [8, Corollary 10]. They have also studied the special case where both the measurable subset and the kernel are invariant under the action of a group [8, Section 4.3]. This case includes compact homogenous manifolds [9].

The methods of Damelin et al. might be used to prove the equidistibution of a sequence of M-codes $\mathscr{X}^*$, where each code X^*_ℓ has the minimum Riesz s-energy of all codes of cardinality $\left|X^*_\ell\right|$. Much care must be taken: although their definition of an admissible kernel includes the Riesz s-kernels as defined in this paper [8, Section 2.1], their definitions and results are framed in terms of sets embedded in Euclidean space, their definition of discrepancy is given in terms of a norm depending on the kernel [8, (8)] and their definition of energy includes the diagonal terms excluded in this paper, so that the energy of the Riesz s-kernel on a finite set is infinite [8, (5) and Section 3].

Brandolini et al. [3, p. 2] give an example where the existence of a partition of the manifold M into N regions, each with volume N^{-1} and diameter at most $cN^{-1/d}$, yields an M-code X obtained by selecting one point from each region, and this gives a bound on the quadrature error of the code X with respect to bounded functions on the manifold M. Such a partition might be constructed by adapting the modified Feige-Schechtman partition algorithm for the unit sphere [10] [16, 3.11.4, pp. 145-148]. Care must be taken to adapt the algorithm, in particular to choose an appropriate radius for the initial saturated packing of the manifold M by balls of a fixed radius. Also, it needs to be proven that the adapted algorithm works for all compact connected Riemannian manifolds and all cardinalities N.

In any case, the existence and construction of equidistributed sequences is only one part of the problem. The sequences relevant to Theorem 1.1 must also be well separated. Further research is needed to address this.

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