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Minimal Discrete Energy Problems and Numerical Integration
on Compact Sets in Euclidean Spaces

by

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Minimal Discrete Energy Problems and Numerical Integration on Compact Sets in Euclidean Spaces

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Summary. In this paper, we announce and survey recent results on (1) point energies, scar defects, separation and mesh norm for optimal $N \geq 1$ arrangements of points on a class of d -dimensional compact sets embedded in \mathbb{R}^n , $n \geq 1$, which interact through a Riesz potential, and (2) discrepancy estimates of numerical integration on the d -dimensional unit sphere S^d , $d \geq 2$.

Keywords and Phrases: Discrepancy, Discrete Riesz Energy, Mesh Norm, Numerical Integration, Point Energies, Riesz Points, Separation, Sphere.

1 Introduction

1.1 Discrete Riesz Energy Problems

The problem of uniformly distributing points on spheres (more generally, on compact sets in \mathbb{R}^n) is an interesting and difficult problem. It is folklore, that such problems were discussed already by Carl Friedrich Gauss in his famous *Disquisitiones arithmeticae*, although it is most likely that similar problems appeared in mathematical writings even before that time.

For $d \geq 1$, let S^d denote the d -dimensional unit sphere in \mathbb{R}^{d+1} , given by

$$x_1^2 + \cdots + x_{d+1}^2 = 1. \quad (1)$$

For $d = 1$, the problem is reduced to uniformly distributing N points on a circle, and equidistant points provide an obvious answer. For $d \geq 2$, the problem becomes much more difficult; in fact, there are numerous criteria for uniformity, resulting in different optimal configurations on the sphere. Many

constructions of “well-distributed” point sets have been given in the literature. These include constructions of generalized spiral points, low-discrepancy point sets in the unit cube, which can be transformed via standard parametrizations, constructions given by integer solutions of the equation $x_1^2 + \dots + x_{d+1}^2 = N$ projected onto the sphere, rotations of certain subgroups applied to points on the sphere, finite field constructions of point sets based on finite field solutions of (1), and associated combinatorial designs. See [2, 5, 13, 14] and the references cited therein.

In this paper, we are interested in studying certain arrangements of N points on a class of d -dimensional compact sets A embedded in \mathbb{R}^n . We assume that these points interact through a power law (Riesz) potential $V = r^{-s}$, where $s > 0$ and r is the Euclidean distance in \mathbb{R}^n .

For a compact set $A \subset \mathbb{R}^n$, $s > 0$, and a set $\omega_N = \{x_1, \dots, x_N\}$ of distinct points on A , the discrete *Riesz s -energy* associated with ω_N is given by

$$E_s(A, \omega_N) := \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-s}. \quad (2)$$

Let $\omega_N^* := \{x_1^*, \dots, x_N^*\} \subset A$ be a configuration, for which $E_s(A, \omega_N)$ attains its minimal value; that is,

$$\mathcal{E}_s(A, N) := \min_{\omega_N \subset A} E_s(A, \omega_N) = E_s(A, \omega_N^*). \quad (3)$$

We shall call such minimizing configurations *s -extremal configurations*. It is well-known that, in general, s -extremal configurations are not always unique. For example, in the case of S^d , they are invariant under rotations. A natural physical interpretation of minimal energy problem on the sphere is the electron problem, which asks for distributions of electrons in stable equilibrium.

Natural questions that arise in studying the discrete Riesz energy are:

- (1) What is the asymptotic behavior of $\mathcal{E}_s(A, N)$, as $N \rightarrow \infty$?
- (2) How are s -extremal configurations distributed on A for large N ?

It is well-known that answers to these questions essentially depend on the relation between s and the Hausdorff dimension $d_H(A)$ of A . We demonstrate this fact with the following two classical examples and refer the reader to [6, 9, 11] and the references cited therein for more details.

Example 1. The interval $[-1, 1]$, $d_H([-1, 1]) = 1$: It is known that $s = 1$ is the critical value in the sense that s -extremal configurations are distributed on $[-1, 1]$ differently for $s < 1$ and $s \geq 1$. Indeed, for $s < 1$, the limiting distribution of s -extremal configurations has an arcsine-type density and, for $s \geq 1$, the limiting distribution is the uniform distribution on $[-1, 1]$. Concerning the minimal energies, they again behave differently for $s < 1$, $s = 1$, and $s > 1$. With $e_s := [\sqrt{\pi}\Gamma(1 + s/2)] / [\cos(\pi s/2)\Gamma((1 + s)/2)]$,

$$\mathcal{E}_s([-1, 1], N) \sim \begin{cases} (1/2)N^2 e_s, & s < 1, \\ (1/2)N^2 \ln N, & s = 1, \\ (1/2)^s \zeta(s) e(s) N^{1+s}, & s > 1, \end{cases}$$

where $\zeta(s)$ stands for the Riemann zeta function.

Example 2. The unit sphere S^d , $d_H(S^d) = d$: Here again, there are three cases to consider: $s < d$, $s = d$, and $s > d$. In all cases, the limiting distribution of s -extremal configurations is given by the normalized area measure σ_d on S^d , which is natural due to rotation invariance, but the asymptotic behavior of $\mathcal{E}_s(S^d, N)$ is quite different. With $\tau_{s,d}(N)$ denoting N^2 if $s < d$, $N^2 \ln N$ if $s = d$, and $N^{1+s/d}$ if $s > d$, the limit $\lim_{N \rightarrow \infty} \mathcal{E}_s(S^d, N)/\tau_{s,d}(N)$ exists and is known in the first two cases (see [5, 8, 9, 11]).

The dependence of the distribution of s -extremal configurations over A and the asymptotics for minimal discrete s -energy on s can be explained using potential theory. Indeed, for a probability Borel measure ν on A , its s -energy integral is defined to be

$$I_s(A, \nu) := \int_{A \times A} |x - y|^{-s} d\nu(x) d\nu(y), \quad (4)$$

which can be finite or infinite. For a set $\omega_N = \{x_1, \dots, x_N\} \subset A$, let

$$\nu^{\omega_N} := \frac{1}{N} \sum_{j=1}^N \delta_{x_j} \quad (5)$$

denote the normalized counting measure of ω_N (so that $\nu^{\omega_N}(A) = 1$). Then the discrete Riesz s -energy (2), associated with ω_N , can be written as

$$E_s(A, \omega_N) = \frac{N^2}{2} \int_{x \neq y} |x - y|^{-s} d\nu^{\omega_N}(x) d\nu^{\omega_N}(y). \quad (6)$$

where the integral represents a discrete analog of the s -energy integral (4).

If $s < d_H(A)$, then it is well-known that the energy integral (4) is minimized uniquely by the *equilibrium measure* ν_s^A . On the other hand, the normalized counting measure $\nu^{\omega_N^*}$ of an s -extremal configuration minimizes the discrete energy integral in (6) over all sets ω_N on A . Thus, one can reasonably expect that, for N large, $\nu^{\omega_N^*}$ is “close” to ν_s^A and, therefore, the minimal discrete s -energy $\mathcal{E}_s(A, N)$ is close to $(1/2)N^2 I_s(A, \nu_s^A)$.

If $s \geq d_H(A)$, then the energy integral (4) diverges for every measure ν . Thus, $\mathcal{E}_s(A, N)$ must grow faster than N^2 . Concerning the distribution of s -extremal points over A , the interactions are strong enough to force points to stay away from each other as far as possible since the closest neighbors are now dominating. So, s -extremal points distribute themselves over A in an equally spaced manner.

In Section 2, we describe some recent results of the authors obtained in [6, 7] concerning separation, mesh norm, and point energies of s -extremal Riesz configurations on a wide class of compact sets in \mathbb{R}^n , and refer the

reader to some latest results of other authors in this area. In particular, we give new separation estimates for the Riesz points on the unit sphere S^d for the case $0 < s < d - 1$ and confirm *scar defects* conjecture ([4, 10]) based on numerical experiments.

1.2 Numerical Integration and g -Functionals

Numerical integration and discrepancy estimates are important problems in applied mathematics and many applications, when one needs to approximate $\int_{\mathcal{B}} f d\zeta$, where $\mathcal{B} \subset \mathbb{R}^n$, $n \geq 3$, is a bounded domain or manifold, $\zeta : \mathbb{R}^n \rightarrow \mathbb{R}$ is a Borel measure with compact support in \mathcal{B} , and f belongs to a suitable class of real valued functions on \mathcal{B} , by a finite sum using values of f at a discrete set of nodes ω_N . Such problems arise naturally in many areas of growing interest such as mathematical finance, physical geodesy, meteorology, and diverse mathematical areas such as approximation theory, spherical t -designs, discrepancy, combinatorics, Monte-Carlo and Quasi-Monte-Carlo methods, finite fields, information based complexity theory, and statistical learning theory.

In this paper, we consider the case when $\mathcal{B} = S^d$ and the measure ζ is the normalized area measure σ_d .

For a set of nodes $\omega_N = \{x_{1,N}, \dots, x_{N,N}\} \subset S^d$, a natural measure for the quality of its distribution on the sphere is the spherical cap discrepancy

$$D(\omega_N) = \sup_{C \subseteq S^d} \left| \sum_{k=1}^N [\nu^{\omega_N} - \sigma_d](C) \right|,$$

where the supremum ranges over all spherical caps $C \subseteq S^d$ and ν^{ω_N} is the normalized counting measure (5) of ω_N . The discrepancy simply measures the maximal deviation between ν^{ω_N} and the normalized area measure σ_d over all spherical caps or, in other words, the worst error in numerical integration of indicator functions of spherical caps using the set of nodes ω_N .

For a continuous function $f : S^d \rightarrow \mathbb{R}$, we denote by

$$R(f, \omega_N) := \int_{S^d} f(x) d\sigma_d(x) - \frac{1}{N} \sum_{k=1}^N f(x_k) = \int_{S^d} f(x) d[\sigma_d - \nu^{\omega_N}]$$

the error in numerical integration on the sphere S^d using nodes in ω_N .

Clearly, to have $R(f, \omega_N) \rightarrow 0$, as $N \rightarrow \infty$, for any continuous function f on S^d , the points in ω_N should be distributed over S^d nicely in the sense that $D(\omega_N) \rightarrow 0$, as $N \rightarrow \infty$.

In Section 3, we briefly discuss spherical cap discrepancy and error estimates for numerical integration on S^d , and refer the interested reader to [5] and the references cited therein for a comprehensive account of this vast and interesting subject. The methods used in [5] are motivated by the discussion on s -energy and s -extremal Riesz points presented in Section 2. A crucial

observation was the possibility of use of g -functionals, generalizing classical Riesz and logarithmic functionals, to estimate the second order terms in the expansions of g -energies, which yield errors in numerical integration valid for a large class of smooth functions on the sphere.

2 Point Energies, Separation, and Mesh Norm for Optimal Riesz Points on d -Rectifiable Sets

In this section, we focus on the results obtained by the authors in [6, 7], which are dealing with properties of s -extremal Riesz configurations on compact sets in \mathbb{R}^n , and refer an interested reader to [8, 9, 10, 11] and references cited therein for results of other authors.

2.1 The case $s > d$

We define a class \mathcal{A}^d of d -dimensional compact sets $A \subset \mathbb{R}^n$ for which, in the case $s \geq d$, the asymptotic behavior of $\mathcal{E}_s(A, N)$, separation and mesh norm estimates, and the limiting distribution of ω_N^* (in terms of weak-star convergence of normalized counting measures) over A have been recently obtained.

Definition 1. *We say that a set A belongs to the class \mathcal{A}^d if, for some $n \geq d$, $A \subset \mathbb{R}^n$ and*

- (1) $H^d(A) > 0$ and
- (2) A is a finite union of bi-Lipschitz images of compact sets in \mathbb{R}^d , that is

$$A = \bigcup_{i=1}^m \phi_i(K_i),$$

where each $K_i \subset \mathbb{R}^d$ is compact and $\phi_i : K_i \rightarrow \mathbb{R}^n$ is bi-Lipschitz on K_i , $i = 1, \dots, m$.

Here and throughout the paper, $H^d(\cdot)$ denotes the d -dimensional Hausdorff measure in \mathbb{R}^n .

For a collection $\omega_N = \{x_1, \dots, x_N\}$ of distinct points on a set $A \subset \mathbb{R}^n$, let

$$\delta(A, \omega_N) := \min_{i \neq j} |x_i - x_j|, \quad \rho(A, \omega_N) := \max_{x \in A} \min_{1 \leq j \leq N} |x - x_j|.$$

The quantity $\delta(A, \omega_N)$ is called the *separation radius* and gives the minimal distance between points in ω_N , while the *mesh norm* $\rho(A, \omega_N)$ means the maximal radius of a “cap” $E(x, r)$ (see (7)) on A , which does not contain points from ω_N . We also define the point energies of the points in ω_N by

$$E_{j,s}(A, \omega_N) := \sum_{i \neq j} |x_j - x_i|^{-s}, \quad j = 1, \dots, N.$$

The following two results were established in [6].

Theorem 1. *Let $A \in \mathcal{A}^d$ and $s > d$. Then, for all $1 \leq j \leq N$,*

$$E_{j,s}(A, \omega_N^*) \leq CN^{s/d}.$$

Corollary 1. *For $A \in \mathcal{A}^d$, $s > d$, and any s -extremal configuration ω_N^* on A ,*

$$\delta(A, \omega_N^*) \geq cN^{-1/d}.$$

We note that this is the best possible lower estimate on the separation radius. Under some additional restrictions on a set $A \in \mathcal{A}^d$, this estimate was obtained earlier in [9]. We also refer the reader to a recent paper [3], where similar results were proved for a *weighted* Riesz energy.

Concerning the mesh norm $\rho(A, \omega_n^*)$ of s -extremal configurations, the following result was proved in [7].

Theorem 2. *Let $A \in \mathcal{A}^d$, $s > d$, and let ω_N^* be an s -extremal configuration on A . Then*

$$\rho(A, \omega_N^*) \leq CN^{-1/d}.$$

Regarding point energies for s -extremal Riesz configurations, we define a subset $\tilde{\mathcal{A}}^d$ of \mathcal{A}^d (see [7]), for which we have obtained a lower estimate matching the upper one in Theorem 1.

Let, for $x \in A$ and $r > 0$,

$$E(x, r) := \{y \in A : |y - x| < r\}. \quad (7)$$

Definition 2. *We say that a set $A \in \tilde{\mathcal{A}}^d$ if*

- (1) $A \in \mathcal{A}^d$ and
- (2) there is a constant $c > 0$ such that, for any $x \in A$ and $r > 0$ small enough,

$$\text{diam}(E(x, r)) \geq cr. \quad (8)$$

Along with trivial examples, such as a set consisting of a finite number connected components (not singletons), the diameter condition holds for many sets with infinitely many connected components. Say, Cantor sets (known to be totally disconnected) with positive Hausdorff measure are in the class $\tilde{\mathcal{A}}^d$.

Theorem 3. *Let $A \in \tilde{\mathcal{A}}^d$ and $s > d$. Then*

$$c \leq N^{1/d} \delta(A, \omega_N^*) \leq C \quad (9)$$

and, therefore, for any $1 \leq j \leq N$,

$$E_{j,s}(A, \omega_N^*) \geq cN^{s/d}. \quad (10)$$

Combining Theorems 1 and 3 yields

Corollary 2. *For $s > d$ and any s -extremal configuration ω_N^* on $A \in \tilde{\mathcal{A}}^d$,*

$$c \leq \frac{\max_{1 \leq j \leq N} E_{j,s}(A, \omega_N^*)}{\min_{1 \leq j \leq N} E_{j,s}(A, \omega_N^*)} \leq C. \quad (11)$$

Thus, for $A \in \tilde{\mathcal{A}}^d$ and $s > d$, all point energies in an s -extremal configuration are asymptotically of the same order, as $N \rightarrow \infty$.

We note that estimates given in Theorems 2, 3, and Corollary 2 were obtained in [6], but with the diameter condition (8) replaced by the more restrictive measure condition $H^d(E(x, r)) \geq cr^d$.

Most likely, (11) is the best possible assertion in the sense that the point energies are not, in general, asymptotically equal, as $N \rightarrow \infty$. (Compare with the case of the unit sphere S^d and $0 < s < d - 1$ in Theorem 4(c) below.)

Simple examples show that the estimates (9), (10), and (11) are not valid, in general, for a set $A \in \mathcal{A}^d$ without an additional condition on its geometry. Indeed, as a counterexample, for $x \in \mathbb{R}^{d+1}$ with $|x| > 1$, let $A = S^d \cup \{x\}$.

2.2 The case $0 < s < d - 1$ for S^d

In doing quadrature, it is important to know some specific properties of low discrepancy configurations, such as the separation radius, mesh ratio, and point energies. In [6], the authors established lower estimates on the separation radius for s -extremal Riesz configurations on S^d for $0 < s < d - 1$ and proved the asymptotic equivalence of the point energies, as $N \rightarrow \infty$.

Theorem 4. *Let ω_N^* be an s -extremal configuration on S^d . Then*

- (a) *for $d \geq 2$ and $s < d - 1$, $\delta(S^d, \omega_N^*) \geq cN^{-1/(s+1)}$;*
- (b) *for $d \geq 3$ and $s \leq d - 2$, $\delta(S^d, \omega_N^*) \geq cN^{-1/(s+2)}$, which is sharp in s for $s = d - 2$;*
- (c) *for any $0 < s < d - 1$,*

$$\lim_{N \rightarrow \infty} \frac{\max_{1 \leq j \leq N} E_{j,s}(S^d, \omega_N^*)}{\min_{1 \leq j \leq N} E_{j,s}(S^d, \omega_N^*)} = 1.$$

We remark that numerical computations for a sphere (see [4, 10]) show that, for any $s > 0$, the point energies are nearly equal for almost all points that are of so-called “hexagonal” type. However, some (“pentagonal”) points have elevated energies and some (“heptagonal”) points have low energies. The transition from points that are “hexagonal” to those that are “pentagonal” or “heptagonal” induce scar defects, which are conjectured to vanish, as $N \rightarrow \infty$. Theorem 4(c) provides strong evidence for this conjecture for $0 < s < d - 1$.

We also refer the reader to a recent paper [12], where sharp separation results for s -extremal configurations are obtained in the case $d - 1 < s < d$.

3 Discrepancy and Errors of Numerical Integration on Spheres.

The following discrepancy and numerical integration results were established in [5].

Definition 3. *Let, for $\delta_0 > 0$, $g(t) : [-1-\delta_0, 1] \rightarrow \mathbb{R}$ be a continuous function. We say that $g(t)$ is “admissible” if it satisfies the following conditions:*

- (a) $g(t)$ is strictly increasing with $\lim_{t \rightarrow 1^-} g(t) = \infty$.
- (b) If $g(t-\delta)$ is given by its ultraspherical expansion $\sum_{n=0}^{\infty} a_n(\delta) P_n^{(d)}(t)$, valid for $t \in [-1, 1]$, then we assume that, for all $n \geq 1$ and $0 < \delta \leq \delta_0$, $a_n(\delta) > 0$.
- (c) The integral

$$\int_{-1}^1 g(t)(1-t^2)^{(d/2)-1} dt$$

converges.

One immediately checks that the following choices of admissible functions $g(t)$ yield the classical energy functionals: $g_L^0(t) := -2^{-1} \log[2(1-t)]$ for the logarithmic energy and $g_R^s(t) := 2^{-s/2}(1-t)^{-s/2}$, $s > 0$, for the Riesz s -energy.

For a set $\omega_N = \{x_1, \dots, x_N\} \subset S^d$, similarly to (2) and (3), we define

$$E_g(S^d, \omega_N) := \sum_{1 \leq i < j \leq N}^N g(\langle x_i, x_j \rangle),$$

where $\langle \cdot \rangle$ denotes inner product in \mathbb{R}^{d+1} , and

$$\mathcal{E}_g(S^d, N) := \min_{\omega_N \subset S^d} E_g(S^d, \omega_N).$$

A point set ω_N^* , for which the minimal energy $\mathcal{E}_g(S^d, N)$ is attained, is called a *minimal g -energy* point set. It was shown in [5] that, for any admissible function $g(t)$, the energy integral

$$I_g(S^d, \nu) := \int_{S^d \times S^d} g(\langle x, y \rangle) d\nu(x) d\nu(y)$$

is minimized by the normalized area measure σ_d amongst all Borel probability measures ν on S^d . Using arguments similar to those in Examples 1 and 2, one expects that the normalized counting measure $\nu^{\omega_N^*}$ of ω_N^* gives a discrete approximation to the normalized area measure σ_d in the sense that the integral of any continuous function f on S^d against σ_d is approximated by the (N^{-1}) -weighted discrete sum of values of f at the points in ω_N^* .

Theorem 5. *Let $g(t)$ be admissible, $d \geq 2$, ω_N be a collection of N points on S^d , f be a polynomial of degree at most $n \geq 1$ on \mathbb{R}^{d+1} , and $0 < \delta \leq \delta_0$. Then*

$$(a) |R(f, \omega_N)| \leq \|f\|_2 \left(\frac{2N^{-2}E_g(S^d, \omega_N) - a_0(\delta) + N^{-1}g(1-\delta)}{\min_{1 \leq k \leq n} [a_k(\delta)/Z(d, k)]} \right)^{1/2}$$

with $Z(d, k)$ counting the linearly independent spherical harmonics of degree k on S^d . Moreover, if $q = q(d)$ is the smallest integer satisfying $2q \geq d + 3$, then there exists a positive constant C , independent of N and ω_N , such that uniformly on $m \geq 1$ and $0 < \delta < \delta_0$ there holds

$$D_N(\omega_N) \leq C \left\{ \frac{1}{m} + \left(\frac{2N^{-2}E_g(S^d, \omega_N) - a_0(\delta) + N^{-1}g(1-\delta)}{\min_{1 \leq k \leq n} [a_k(\delta)/Z(d, k)]} \right)^{1/2} \right\}.$$

(b) Let f be a continuous function on S^d satisfying

$$|f(x) - f(y)| \leq C_f \arccos(\langle x, y \rangle), \quad x, y \in S^d. \quad (12)$$

Then, for any $n \geq 1$,

$$|R(f, \omega_N)| \leq 12C_f \frac{d}{n} + \left(\frac{2N^{-2}E_g(S^d, \omega_N) - a_0(\delta) + N^{-1}g(1-\delta)}{\min_{1 \leq k \leq n} [a_k(\delta)/Z(d, k)]} \right)^{1/2}.$$

Remark 1. (a) Theorem 5 shows that second order terms in the expansion of minimal energies determine rates in errors of numerical integration over spheres. Indeed, one hopes that the energy term $2N^{-2}E_g(S^d, \omega_N)$ and the leading term $a_0(\delta)$ cancel each other sufficiently to allow for an exact error. An application of this idea was exploited first in [5] in the case $s = d$. (See Theorem 6 below.)

(b) Brauchart [1] has considered invariance principles for energy functionals based on Theorem 5, which allow for a family of g -functionals to conclude that for any s -extremal configuration on S^d , $0 < s < d$, $R(f, \omega_N^*) \rightarrow 0$, as $N \rightarrow \infty$, and this error can be explicitly calculated due to the finiteness of the corresponding energy integral.

(c) The fact that the error in Theorem 5 goes to zero for any s -extremal configuration (without rate of convergence) follows from the finiteness of the energy integral ($0 < s < d$), Theorem 6 below ($s = d$), and results of [8] and [9] ($s \geq d$).

We now quantify the error in Theorem 5 for d -extremal configurations on S^d (which are sets of minimal g_R^d -energy).

Theorem 6. *Let f be a continuous function on S^d satisfying (12), and let ω_N^* be a d -extremal configuration. Then*

$$|R(f, \omega_N^*)| = \mathcal{O} \left(\frac{C_f + \|f\|_\infty \sqrt{\log \log N}}{\sqrt{\log N}} \right)$$

with the implied constant depending only on d . Moreover,

$$D(\omega_N^*) = \mathcal{O}\left(\sqrt{\log \log N / \log N}\right).$$

We remark that it is widely believed that the order above may indeed be improvable to a negative power of N . Thus far, however, it is not clear how to prove whether this belief is indeed correct.

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