Project description

1 Introduction

We propose to develop theoretical and numerical tools necessary to study attractive-repulsive interactions of N particles. Such interactions arise in models of biological, economical, and physical systems. The longest-scale counterpart of the discreteness phenomena described below is the clustering of galaxies, which has been the focus of the cosmological community for the past few decades. In the present disposition we shall start by discussing the Riesz s-energies and their applications, to illustrate usefulness of the theory of the corresponding minimizers. We further consider the p-frame energy interactions on the sphere, and their connections to spherical designs.

Understanding simple attractive-repulsive energies such as the above will serve as a step towards more complex interactions, corresponding to highly non-convex functionals on the phase space. Examples include molecular system interactions, magnetic interactions within antiferromagnets, causal variational principles, and other functionals arising in computational physics.

A large part of this proposal deals with the set-up of numerical simulations of the equilibrium measures for p-frame interactions. It is clear that a theory of N-body interaction minimizers that would be applicable to a wide class of kernels and underlying sets is impossible. This underlines the importance of precise numerical studies of such large non-convex systems. Based on the collaboration started at the 2018 semester program at ICERM, "Point Configurations in Geometry, Physics and Computer Science", the PI suggests a study of non-positive definite energies on the sphere, especially the p-frame energy.

2 Results from prior support

As a graduate student, the PI was supported, in part, by the National Science Foundation grants of Edward Saff and Douglas Hardin: DMS-1412428, DMS-1516400, and DMS-1521749. This research resulted in papers [HSV17, RSV17, VMFF18].

In the context of N-body interactions given above, the Riesz kernel considered in this section is an example of a strongly-repulsive kernel, and therefore does not exhibit clustering. The following description of previous research is given as an illustration of usefulness of the energy framework, as well as of some of the computational challenges arising in it.

Intellectual merit. The so-called Riesz s-kernel $\|x-y\|^{-s}$ gives an example of a strongly-repulsive interaction. It has been shown that pairwise interaction energies with Riesz kernels have properties making them suitable for applications to numerical integration, finite difference schemes, and computational geometry [HSV17, VMFF18]. It was therefore important to develop methods allowing to generate large near-minimizing configurations with low computational cost. Similar methods can be used to approximate a given smooth distribution with discrete configurations. It remarkable that the cited methods are applicable to arbitrary ambient dimension under mild smoothness assumptions on the underlying set.

Broader impacts. Theorems 1–4 below provide a tool for discretization of measures with continuous density functions (with respect to the Hausdorff measure on a manifold). The resulting discrete measures will have optimal orders of local separation and covering on the manifold, and are therefore well suited for diverse applications: surface modelling, RBF-FD solvers, sensor deployment, etc. An algorithm for node distribution in subsets of $\mathbb{R}^d$ with nonempty interior was developed and implemented in [VMFF18]; it is shown below as Algorithm 1. We have collected numerical evidence [VMFF18, Section 5.1] that the resulting nodes give better-conditioned systems for interpolation with PHS-based (polyharmonic spline) RBF kernels than Halton nodes or nodes on the Cartesian grid.

2.1 Discretization with minimizers of Riesz-based functionals

We refer to lower semicontinuous functions from the Cartesian product $\Omega^N \subset (R^D)^N$ to $\mathbb{R}$ as *energies*, to reflect their physical interpretation. Notice that in the following $\|\cdot\|$ always denotes the Euclidean norm in $\mathbb{R}^D$. Expression $C_{s,d}$ stands for a universal constant, depending only on s and d. The exact value of this

constant is when for $s = d$ or $d = 1, 8, 24$, and conjectured for some other pairs (s, d) [BHS12, CKM+19]; computational value of $C_{s,d}$ can be readily obtained by minimizing the Riesz energy for a given pair s, d.

Based on earlier work of Hardin and Saff [HS05], together with them the PI has obtained several results about the asymptotic behavior of minimizers of a class of discrete energies, when the number of particles $N \to \infty$. The considered energies are based on the Riesz kernel $g_s(x, y) := \|x - y\|^{-s}$. For a lower semicontinuous function q, define the discrete Riesz energy by

$$(\star) \qquad E_s(\cdot\,; q){:}(x_1, \dots, x_N) \in \Omega^N \mapsto \sum_{i \neq j} g_s(x_i, x_j) + \tau(N) \sum_i q(x_i),$$

where the scaling factor $\tau(N)$ is given by

$$(1) \qquad \tau(N) = \tau_{s,d}(N) := \begin{cases} N, & s < d := \dim_H \Omega, \\ N \log N, & s = d, \\ N^{s/d}, & s > d. \end{cases}$$

We shall further write $\omega_N := \{x_1, \dots, x_N\}$ and, accordingly, $E_s(\omega_N; q)$ in place of $(\star)$. In the case $s = D - 2$, $E_s(\omega_N; q)$ corresponds to the energy of electrostatic interaction of particles $x_1, \dots, x_N$. In what follows we deal primarily with the so-called hypersingular case $s \geq d = \dim_H \Omega$, the Hausdorff dimension of Ω. We shall also need to characterize smoothness of the underlying set Ω as follows.

Definition 1. The set $\Omega \subset \mathbb{R}^D$ is called *d-rectifiable* if there exists a compact set $\mathcal{C} \subset \mathbb{R}^d$ and a Lipschitz map $\eta : \mathbb{R}^d \to \mathbb{R}^D$ such that $\eta(\mathcal{C}) = \Omega$.

Furthermore, Ω is *d-regular* with respect to the Hausdorff measure $\mathcal{H}_d$, if there exists a positive constant c, such that for every r, $0 < r \leqslant \operatorname{diam} \Omega$, and every $x \in \Omega$,

$$(2) \qquad c^{-1} r^d \leqslant \mathcal{H}_d(\Omega \cap B(x, r)) \leqslant c r^d.$$

Asymptotic behavior of the energy E_s for $N \to \infty$ is described by the following result.

Theorem 1. *[HSV17] Assume that $s > d$, the compact set Ω is d-rectifiable, and $\mathcal{H}_d(A) > 0$. Let further $L_1 = L_1(q, \Omega)$ be the (unique) constant such that*

$$d\mu_q := \left(\frac{L_1 - q(x)}{C_{s,d}(1 + s/d)} \right)_+^{d/s} d\mathcal{H}_d$$

is a probability measure on Ω. Then every sequence $\tilde{\omega}_N$, $N \geq 2$, of minimizers of the functional $E_{s,d}(\cdot\,; q)$ on Ω^N, $N \geq 2$, satisfies

$$\lim_{N \to \infty} \frac{E_{s,d}(\tilde{\omega}_N; q)}{N^{1+s/d}} = \int \frac{L_1 d + q(x) s}{d + s} \, d\mu_q(x) =: S(q, \Omega).$$

The above theorem shows in particular that the assumption of compactness of Ω is non-essential, and can be replaced with compactness of sublevel sets of q. The physical interpretation of this fact is that the external field q can serve as an energy well confining the particles.

It is also established in [HSV17] that the weak* limit of counting measures of sequences with optimal asymptotic of $(\star)$ is necessarily $d\mu_q$:

Theorem 2. *[HSV17] For any sequence ω_N, $N \geq 2$,*

$$\lim_{N \to \infty} \frac{E_{s,d}(\omega_N; q)}{N^{1+s/d}} = S(q, \Omega)$$

implies

$$\frac{1}{N} \sum_{x \in \omega_N} \delta_x \xrightarrow{*} d\mu_q \quad \text{as } N \to \infty.$$

The uniqueness result in the last theorem is an indication that with $N \to \infty$, the energy E_s as a functional on the space of discrete configurations is in a certain sense convex. Indeed, an appropriate notion of convergence makes this convexity evident.

Definition 2. [DGF75, DG06, p. 517] Let X be a metric space. Suppose that the functionals F, $F_n : X \to \mathbb{R} \cup \{+\infty\}$, $n \geq 1$, satisfy

1. for every sequence $\{x_n\} \subset X$ such that $x_n \to x$, $n \to \infty$, there holds
$$\liminf_{n\to\infty} F_n(x_n) \geq F(x);$$
2. for every $x \in X$ there exists a sequence $\{x_n\} \subset X$ converging to it and such that
$$\lim_{n\to\infty} F_n(x_n) = F(x).$$

Then we say that the sequence $\{F_n\}$ is Γ-*converging* to the functional F; in symbols, $F_n \xrightarrow{\Gamma} F$.

In our case $X = \mathcal{P}(\Omega)$, the space of probability measures on Ω, equipped with weak* topology (metrizable on a compact Ω). For the rest of this section we shall pass to more general energies:

$$E_s(x_1, \dots, x_N; \kappa, q) := \sum_{i\neq j} \kappa(x_i, x_j) g_s(x_i, x_j) + \tau(N) \sum_i q(x_i), \tag{3}$$

where the function $\kappa : \Omega \times \Omega \to \mathbb{R}$ is continuous at the points of the diagonal, $\operatorname{diag}(\Omega \times \Omega)$, in the product topology. Through the identification of discrete subsets of Ω with their counting measures, the energy (3) acts on a proper subset of $\mathcal{P}(\Omega)$; we now consider its extension to the whole space $\mathcal{P}(\Omega)$ of probability measures on Ω:

$$\frac{1}{\mathcal{T}(N)} E_{s,N}(\mu; \kappa, q) := \begin{cases} \frac{1}{\mathcal{T}(N)} E_s(\{x \,:\, x \in \operatorname{supp}\mu\}; \kappa, q) & \text{if } \mu \in \mathcal{P}_N(\Omega), \\ +\infty, & \text{otherwise,} \end{cases} \tag{4}$$

where

$$\mathcal{P}_N(\Omega) := \{\mu \in \mathcal{P}(\Omega) : \#(\operatorname{supp}\mu) = N\}.$$

The Γ-limit of the sequence $E_{s,N}$ is described by the following functional on $\mathcal{P}(\Omega)$:

$$G_s(\mu; \kappa, q) := \begin{cases} C_{s,d} \int_\Omega \kappa(x,x) \varphi(x)^{1+s/d} d\mathcal{H}_d(x) + \int_\Omega q(x)\varphi(x) d\mathcal{H}_d(x), & \mu = \varphi d\mathcal{H}_d, \\ +\infty, & \text{otherwise.} \end{cases} \tag{5}$$

Theorem 3. *[Vla18] Suppose Ω is d-rectifiable. If κ is continuous at every $(x,x) \in \operatorname{diag}(\Omega \times \Omega)$, q is continuous on Ω, and g_s is the Riesz kernel with $s > d$, then*

$$\frac{1}{\mathcal{T}(N)} E_N(\cdot\,; g_s, \kappa, q) \xrightarrow{\Gamma} G_s(\cdot; \kappa, q), \qquad N \to \infty, \tag{6}$$

on $\mathcal{P}(\Omega)$ equipped with the weak* topology.

Notice that G_s is convex on $\mathcal{P}(\Omega)$; since the minimum of a Γ-limit is a lower bound for minima of the elements of the sequence, this gives an easy proof Theorem 2. In addition, applying a calculus of variations argument to G_s gives the density of the limiting measure of minimizers of (3) with respect to the Hausdorff measure:

$$\varphi^{\kappa,q}(x) = \frac{d\mu^{\kappa,q}}{d\mathcal{H}_d}(x) := \left(\frac{L_1 - q(x)}{C_{s,d}(1 + s/d)\kappa(x,x)} \right)_+^{d/s},$$

where L_1 is a chosen so that $\mu^{\kappa,q}(\Omega) = 1$. This shows a very natural connection between the two modifications of the original hypersingular Riesz energy, using the multiplicative weight, and an external field term, and allows to work with their combination.

Lastly, the local behavior of the minimizers is summarized in the following statement, where $\Omega(L) = \{x \in \Omega : q(x) \leqslant L\}$ is an L-sublevel set of function q, and $\operatorname{dist}(x, \tilde{\omega}_N) = \min\{\|x - y\| : y \in \tilde{\omega}_N\}$ is the distance from vector x to the set $\tilde{\omega}_N$.

Theorem 4. *[HSV17] For every sequence of minimizers $\tilde{\omega}_N$, $N \geq 2$, there exists a constant C_1 such that*

$$\min\left\{\|x-y\| : x \neq y;\ x, y \in \tilde{\omega}_N\right\} \geq C_1 N^{-1/d}.$$

If, in addition to the rectifiability assumption, the set Ω is also d-regular, then for each $h > 0$ there is a constant C_2, such that every $x \in \Omega(L_1 - h)$ satisfies

$$\operatorname{dist}(x, \tilde{\omega}_N) \leqslant C_2 N^{-1/d}.$$

The local separation property applies also to the nodes constructed by the Algorithm 1 in the following section.

2.2 Practical node distribution algorithm

Theorems 1–4 give a way to construct discrete configurations approximating a given smooth measure on the underlying set Ω. However, it is a well-known experimental observation that the number of local minima of the Riesz energies grows exponentially with the number of points N [EH07]. In view of this fact, finding exactly even local minimizers for such a problem can be a formidable task. It is strictly necessary to produce exact minimizers in order to approximate a given distribution? We shall give a partial answer to it in this section, by giving a fast procedure, based on the gradient of the Riesz energy, that generates nodes in the time close to $O(N \log N)$ in the total number of nodes (assuming that the target density can be evaluated in the time, linear in N).

For a node set $\omega = \{x_1, \ldots, x_N\} \subset \Omega$, we need the following notations:

$$\Delta(x) := \min\{\|y - x\| : y \in \omega \text{ and } y \neq x\}$$

and

$$\Delta(\omega) := \min\{\Delta(x) : x \in \omega\}.$$

Suppose that the node density is prescribed by $\rho : \Omega \to [0\,, \infty)$ so that there must hold

$$\Delta(x) \asymp \rho(x), \qquad x \in \omega,$$

with equivalence constants independent of x. Algorithm 1 for distributing nodes according to the given density, developed by the PI together with Bengt Fornberg, Natasha Flyer, and Timothy Michaels, is also fully applicable if the node distribution is prescribed by a volumetric density (number of particles per unit volume).

To demonstrate scalability of our implementation, we used the geodata [AE09] from the collection of global relief datasets produced by NOAA (National Oceanic and Atmospheric Administration), which contains a 1 arc-minute resolution model of Earth. We generate a sample configuration consisting of 1,356,566 nodes distributed uniformly inside an atmospheric-type shell: the outer boundary of the shell is spherical, the inner one is an interpolation of the relief from $ETOPO1$ data, exaggerated by a factor of 100.

The right image in Figure 1 shows node distribution close to the boundary; notice that there are no "holes" forming. Specifically, we have verified that the Voronoi radii of the resulting configuration are smaller than the nearest neighbor distances, so no additional nodes can be introduced without decreasing the separation distance. This means, the set Ω is packed with nodes in an efficient way.

Instead of computing the exact minimizers of the energies $(\star)$, we suggest moving a quasi-Monte Carlo sequence, approximating ρ, with a gradient-type flow obtained from the truncated Riesz energy. A general iteration has the form

$$g_i^{(t)} = s\,\rho\left(\boldsymbol{x}_i^{(t)}\right)^s \sum_{k=1}^{K} \frac{\boldsymbol{x}_i^{(t)} - \boldsymbol{x}_{j(i,k)}^{(t)}}{\|\boldsymbol{x}_i^{(t)} - \boldsymbol{x}_{j(i,k)}^{(t)}\|^{s+2}}, \quad 1 \leqslant i \leqslant N.$$

Here $\boldsymbol{x}_{j(i,k)}^{(t)}$, $1 \leqslant k \leqslant K$, are the K nearest neighbors of $\boldsymbol{x}_i^{(t)}$; $t, 1 \leqslant t \leqslant T$ denotes the number of the iteration. Each node is moved by a fixed fraction of the nearest neighbor distance:

$$\boldsymbol{x}_i^{(t+1)} = \begin{cases} \boldsymbol{x}_i^{(t)} + \dfrac{\Delta\left(\boldsymbol{x}_i^{(t)};\, \omega_N^{(t)}\right)}{t + C} \dfrac{g_i^{(t)}}{\|g_i^{(t)}\|} & \text{if this sum is inside } \Omega; \\ \boldsymbol{x}_i^{(t)}, & \text{otherwise,} \end{cases} \qquad 1 \leqslant i \leqslant N.$$

Algorithm 1: 3dRBFnodes [VMFF18]

Data: radial density ρ; indicator function $\mathbb{1}_\Omega$
Result: nodes $x_1, \ldots, x_N$ with nearest neighbor distance $\Delta(x_i) \asymp \rho(x_i)$
begin

$\mathcal{T} \leftarrow \emptyset$ // distance look-up table
$\omega \leftarrow \emptyset$ // node set
$\sigma \leftarrow +\infty$; $m \leftarrow 1$
while $\sigma > \min_\Omega \rho$ **do**
  $\sigma \leftarrow \Delta(\mathcal{M}_m)$ // $\mathcal{M}_m$ is m-point quasi-Monte Carlo set
  $\mathcal{T} \leftarrow \mathcal{T} \cup \{s\}$ // tabulate separation distances
  $m \leftarrow m + 1$
$\lambda \leftarrow \mathcal{T}^{-1}$ // inverse map to the look-up table
2 $\{\mathcal{V}_m : m \in \mathcal{D}\}$ // voxels adjacent to support
for $m \in \mathcal{D}$ **do**
  $V \leftarrow$ vertices of $\mathcal{V}_m$
  $\bar{\rho}_m \leftarrow \langle \rho(V) \rangle$ // $\langle \cdot \rangle$ denotes mean value
  $n_m \leftarrow \lambda(\bar{\rho}_m)$
  $\omega \leftarrow \omega \cup \{c_m + h_m + f_m \mathcal{M}_{n_m}\}$ // offset and rescale at insertion
3 $\{\mathcal{V}_m : m \in \mathcal{D}\}$ // empty voxels
for $m \in \mathcal{E}$ **do**
  if $\Delta(z_m) > \rho(z_m)$ // z_m is the m-th center
  then
    $\omega \leftarrow \omega \cup \{z_m\}$ // saturate remaining voxels
4 **for** $x \in \omega$ **do**
  if $\mathbb{1}_\Omega(x) = 0$ **then**
    delete x // remove points outside support
5 **for** $t \in 1 \ldots T$ **do**
  for $x \in \omega$ **do**
    $g \leftarrow 0$
    for $x_k \in$ nearest neighbors of x **do**
      $g \leftarrow g + s\rho(x)^s \frac{x - x_k}{\|x - x_k\|^{s+2}}$
    $dx \leftarrow \frac{\Delta(x)}{t + C} \cdot \frac{g}{\|g\|}$
    $x \leftarrow \text{pullback}(x + dx)$

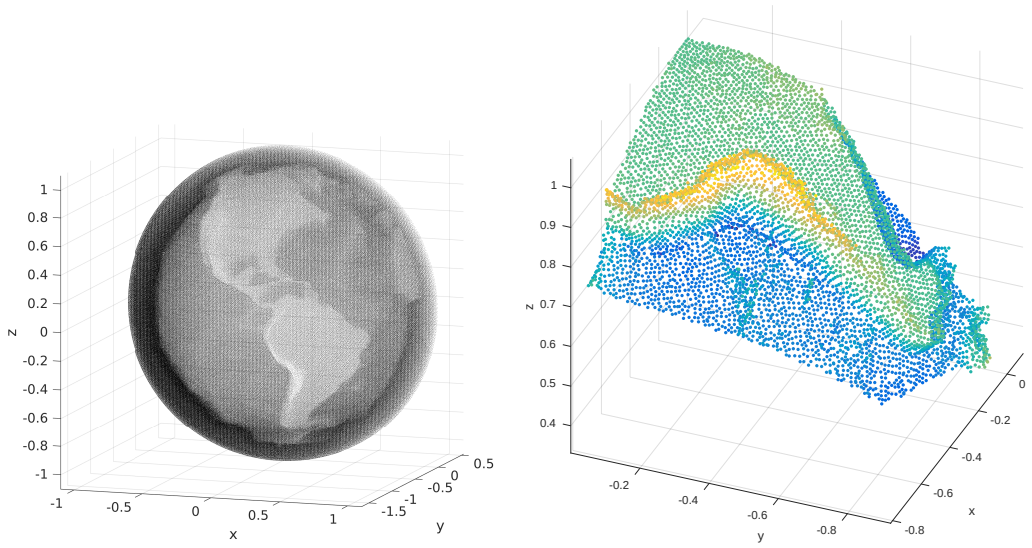

Figure 1: A node set shaped as an atmospheric layer over the Western hemisphere, and a fragment of the Western coast of South America, color-coded by altitude.

The multiplicative approach is employed to reduce the computational complexity of the algorithm, and the theoretic groundwork is provided by [BHS14]. The outlined procedure is very efficient; for example, a simple implementation in Matlab [VM17] without parallelization handles up to at least 3 million nodes on a standard PC.

3 Intellectual merit

This section gives the relevant background on attractive-repulsive potentials and formulates the goals of the present proposal. Such interactions are different from the Riesz kernel-interaction, discussed above, as they are continuous at the origin, allowing clustering of interacting charges. However, the lack of strong singularity at the origin means that approximate minimizers cannot be constructed with the truncated gradient flow described in Section 2.2. Instead, it is necessary to deal with the complete nonlocal N-body interaction; we shall further discuss the computational challenges of this problem in Section 3.2.

3.1 Minima of quadratic functionals on probability measures

We consider a fixed underlying set Ω; for simplicity in this section it can be assumed that $\Omega = \mathbb{S}^d$, the unit sphere in $\mathbb{R}^{d+1}$, although all the essential aspects of the following discussion apply to any compact connected 2-point homogeneous space as well (such spaces include spheres and projective spaces over normed division algebras on $\mathbb{R}$ [Wan52]). We are also interested in generalizing the following results to other smooth manifolds.

We shall focus on functionals I acting on the space of probability measures $\mathcal{P}(\Omega)$ in the following way:

$$I_f(\mu) := \iint\limits_{\mathbb{S}^d} f(\|x-y\|)\, d\mu(x) d\mu(y).$$

The given quantity describes self-interaction energy of the measure μ; every pair of elements in $\operatorname{supp}\mu$ contributes to the value of this energy. Non-local interactions of this form are used to model various physical, biological, and economical interactions: molecular forces, biological swarms, gravitational forces, etc. [BCLR13, CCH14, CCP15, CFP17]. Our primary goal in dealing with such functional is identifying salient of the measures minimizing $I_f(\mu)$; we are especially interested in cases when such measures can be described completely, but more generally we would like to understand the shape of their supports, whether they are discrete, etc.

Of course, on the sphere functional I_f is equivalent to a functional with the kernel that depends only on the scalar product $x \cdot y$:

$$I_f(\mu) = \iint\limits_{\mathbb{S}^d} f(x \cdot y)\, d\mu(x) d\mu(y). \tag{7}$$

Given a lower semicontinuous kernel f, expression (7) defines a functional on $\mathcal{P}(\Omega)$, lower semicontinuous in the weak* topology. Since $\mathcal{P}(\Omega)$ is compact, the problem of finding measures minimizing (7) is well-defined. Observe further that it is possible to extend this setting to the case of unbounded Ω, provided that the kernel f confines minimizers to a compact set. In fact, the paper of Carrillo, Figalli, and Patacchini [CFP17] considers the problem of minimizing

$$E_W(\mu) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(\|x - y\|) d\mu(x) d\mu(y)$$

over all probability measures $\mathcal{P}(\mathbb{R}^d)$, assuming that W satisfies certain growth conditions:

1. $W(0) = 0$
2. $W(r) < 0$ for $0 < r < R$ for some R
3. $W(r) \geq 0$ otherwise
4. For an $\alpha > 1$,
$$W'(r) r^{-\alpha} \to -C, \qquad r \to 0+$$

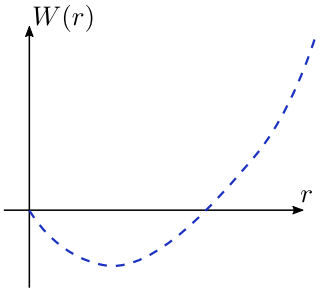

Figure 2: Profile of a radial attractive-repulsive force.

Under these conditions Carrillo et al. established the following.

Theorem 5 ([CFP17]). *The global minimizer of E_W over $\mathcal{P}(\mathbb{R}^d)$ is discrete.*

Goal 1. *Identify the correct generalization of Theorem 5 to optimization over measures in $\mathcal{P}(\Omega)$, supported on a smooth manifold Ω.*

Conjecture 1.1. *A similar result holds with repulsive kernels, on manifolds with non-vanishing Gaussian curvature.*

Apart from the general setting given above, it is important from the point of view of computational geometry to consider the following so-called *p-frame kernel*. Let $f_p(t) = |t|^p$ with $p > 0$. Writing $\mathbb{S}^d$ for the d-dimensional unit sphere, consider the discrete and continuous energy with the kernel f_p:

$$I_p(x_1, ..., x_N) := \frac{1}{N^2} \sum_{i,j=1}^{N} |x_i \cdot x_j|^p \quad \text{and} \quad I_p(\mu) := \iint\limits_{\mathbb{S}^d} |x \cdot y|^p \, d\mu(x) d\mu(y).$$

To explain the motivation behind this energy, we shall first introduce the notion of a frame.

Definition 3. $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^{d+1}$ is a *frame* if there exist constants $0 < A \leqslant B < \infty$ such that

$$A\|y\|_2^2 \leqslant \sum_{k=1}^{N} |y \cdot x_k|^2 \leqslant B\|y\|_2^2$$

for all $y \in \mathbb{R}^{d+1}$.

A frame is called *tight* if

$$\sum_{k=1}^{N} |y \cdot x_k|^2 = A\|y\|_2^2$$

for all $y \in \mathbb{R}^{d+1}$; the quantity A is then called the *frame constant*.

Note the similarity between the last display and the Parseval identity. Indeed, intuitively, frame is a basis with redundancy. For example, if $\{e_1, \dots, e_{d+1}\}$ is a collection of basis vectors in $\mathbb{R}^{d+1}$, then for any set of orthogonal matrices $O_1, \dots, O_K$, the collection of $K(d+1)$ vectors $\{O_k e_1, \dots, O_K e_{d+1}\}_{k=1}^K$ is a tight frame with the frame constant K. Such configurations are useful in applied harmonic analysis, since encoding with respect to a frame instead of a basis allows for increased robustness of the signal; recovery of the encoded information is possible even for lossy transmission.

An important characterization of tight frames, obtained by Benedetto and Fickus [BF03], is that they minimize the 2-frame energy, $I_2(\mu)$, over the set of counting measures supported on N vectors, which we denote by $\mathcal{P}_N(\mathbb{S}^d)$:

$$\mathcal{P}_N(\mathbb{S}^d) = \left\{ \frac{1}{N} \sum_{i=1}^N \delta_{x_i} : x_1, \dots, x_N \in \mathbb{S}^d \right\} \simeq (\mathbb{S}^d)^N.$$

Theorem 6 ([BF03])**.** *Minimizers of $I_2(\mu)$ over measures in $\mathcal{P}_N(\mathbb{S}^d)$ are*

1. *orthonormal sequences if $N \leqslant d$;*
2. *tight frames if $N \geq d$.*

Furthermore, functional I_2 is minimized on every measure with the second moment matrix proportional to the identity matrix, that is, if the following matrix equality holds:

$$\left(\iint_{\mathbb{S}^d} x_i x_j \, d\mu(x) \right)_{i,j} = c \mathbb{1}_{d+1}.$$

It is therefore a natural question to ask what are the minimizers of I_p for other values of p; can any other remarkable configurations obtained in this way? Before answering this question in the positive, we need to make precise what it means for a configuration to be "remarkable". We start by defining equal-weight spherical quadratures, exact for polynomials up to a certain degree.

Definition 4. We say that a discrete set $\mathcal{C} \subset \mathbb{S}^d$ is a *spherical design of degree k*, if for any polynomial p of degree at most k, there holds

$$\int_{\mathbb{S}^d} p(x) d\sigma_d(x) = \frac{1}{N} \sum_{x \in \mathcal{C}} p(x),$$

where σ_d is the uniform measure on $\mathbb{S}^d$.

The linear programming (LP) methods that we shall now discuss apply to an even more special class of configurations, a very special class of designs.

Definition 5. A discrete set $\mathcal{C} \subset \mathbb{S}^d$ is a *tight design*, if one of the following conditions holds:

1. $\mathcal{C}$ is a design of degree $2m-1$ and there are m distances between its distinct elements, including an antipodal pair;
2. $\mathcal{C}$ is a design of degree $2m$ and there are m distances between its distinct elements.

This definition can be naturally generalized to other 2-point homogeneous compact spaces.

Using the methods of linear programming, the PI and coauthors: Dmitriy Bilyk, Alexey Glazyrin, Ryan Matzke, and Josiah Park [BGM+19b], have recently established that tight designs minimize I_p. The LP framework can be concisely summarized as a sequence of inequalities:

$$I_f(\mu) \geq I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma_d) = I_{H[f,g]}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}).$$

Here $H[f,g]$ denotes the Hermite interpolant of the kernel f, agreeing with it at the values of scalar products $x \cdot y$ occurring in $\mathcal{C}$; g stands for the polynomial vanishing on these scalar products. The first inequality follows from $H[f,g] \leqslant f$, a property of the Hermite interpolant; the second is due to positive-definiteness of

the interpolant [BGM+19b, CK07]. The two equalities are, respectively, due to $\mathcal{C}$ being an exact quadrature for polynomials of degree up to $\deg H[f,g]$, and the fact that $H[f,g]$ and f coincide in at the scalar products in $\mathcal{C}$, as already mentioned. To summarize, all the inequalities can be replaced with equalities if and only if $\mathcal{C}$ is a tight design; this is the result of the following theorem.

Theorem 7. *[BGM+19b] If $f^{(k)} \geq 0$ for $0 \leqslant k \leqslant M$, but $f^{(M+1)} \leqslant 0$ in $(-1,1)$, and $\mathcal{C}$ is a tight spherical design of degree M, then*

$$\mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is the unique global minimizer of

$$I_f(\mu) = \iint_{\mathbb{S}^d} f(x \cdot y)\, d\mu(x) d\mu(y)$$

over $\mathcal{P}(\Omega)$.

Now let us recall some familiar configurations which are tight designs (more can be found in the Table 1).

Corollary 1. *[BGM+19b] The minimizer of $F_p(\mu)$ on $\mathbb{S}^2$ for $p \in (2,4)$ is supported on the regular inscribed icosahedron.*

Corollary 2. *[BGM+19b] The minimizer of $F_p(\mu)$ on $\mathbb{S}^{23}$ for $p \in (8,10)$ is supported on the shortest vectors of the Leech lattice, normalized to the unit sphere.*

d	$N/2$	Upper bound on I_p	Range of p	Tight	Name
2	$N/2$	*	$[2N-4, 2N-2]$	T	regular $2N$-gon
3	6	0.241202265916660	$[2,4]$	T	icosahedron
3	11	0.142857142857143	$6-$		Reznick design
3	16	0.124867143799450	$[6,8]$		icosahedron + dodecahedron
4	11	0.125000000000000	$4-$		small weighted design
4	24	0.096277507157493	$[4,6]$		D_4 root vectors
4	60	0.047015486159502	$[8,10]$	C	600-cell
5	16	0.118257675970387	$[2,4]$		hemicube
5	41	0.061838820473855	$[4,6]$		Stroud design
6	22	0.090559619406078	$[2,4]$		cross-polytope + hemicube
6	63	0.042488105634495	$[4,6]$		E_6 & E_6^* roots
7	28	0.071428571428571	$[2,4]$	T	kissing E_8
7	91	0.030645893660944	$[4,6]$		E_7 & E_7^* roots
8	36	0.059098639455782	3		mid-edges of regular simplex
8	120	0.022916666666667	$[4,6]$	T	E_8 roots
23	276	0.011594202898551	$[2,4]$	T	equiangular lines
23	2300	0.002028985507246	$[4,6]$	T	kissing Leech lattice
24	98280	0.000103419439357	$[8,10]$	T	Leech lattice roots

Table 1: Optimal and conjectured optimal configurations for p-frame energies on $\mathbb{RP}^{d-1}$. For interval ranges of p, bounds concern the value of p equal to the midpoint. Λ^* denotes the lattice dual to Λ. Note that in the cases denoted by "T", Theorem 7 gives that the corresponding upper bound is exact. For the 600-cell we have obtained a computer-assisted proof of optimality, shown above by "C". All the shown digits are exact, and were obtained by the custom optimization package discussed in Section 3.2.

In order to explain why the uniform measure σ_d is no longer a minimizer for p non-even, we shall need to introduce some classical definitions going back to Schoenberg. Namely, recall the notion of positive-definiteness [Sch41]:

Definition 6. The function $f : \mathbb{S}^d \mapsto \mathbb{R}$ is called *positive definite on* $\mathbb{S}^d$, if for every collection of vectors $\{x_1, \dots, x_N\} \subset \mathbb{S}^d$ and arbitrary real $c_1, \dots, c_N$,

$$\sum_{i,j=1}^{N} f(x_i \cdot x_j) c_i c_j \geq 0.$$

It is due to Schoenberg himself (established in the cited paper) that on the unit sphere $\mathbb{S}^d$, positive-definiteness is equivalent to having nonnegative Fourier coefficients in terms of Gegenbauer polynomials. It turns out that I_f is minimized on σ_d if and only if f is positive-definite, which is the case of p-frame energy only for even p. Still there is no exhaustive answer to the following question.

Goal 2. *How is the positive-definiteness of the kernel related to the cardinality or absolute continuity of its minimizers?*

Due to the results of Horn and Fitzgerald-Horn [Hor69, FH77], and the argument of Björck [Bjö56], behavior of the minimizer of given p-frame potential appears to be related to the positive-definiteness of the matrix $H := (|x_i \cdot x_j|)_{i,j}$, obtained from the Gram matrix of the configuration by taking absolute values of every entry. We have collected substantial numerical evidence corroborating the following statement, which appears related to the result of Theorem 8.

Conjecture 2.1. *For any dimension d, there exists a value $N(d)$ for which the Hadamard-absolute value H of the Gram matrix of an optimal code $\mathcal{C}_0$ is positive definite if and only if the number of vectors in the code satisfies $\#\mathcal{C}_0 \leqslant N(d)$.*

Here for any given cardinality N, the optimal code is the configuration of N vectors on $\mathbb{S}^d$, maximizing the minimal separation distance (equivalently, solving the best-packing problem in geodesic distance).

Studying minimizer of the p-frame potential may give information about the existence of maximal equiangular tight frames (ETFs) in higher dimensions. Recall that an ETF is a discrete configuration $\mathcal{C} = \{x_k\} \subset \mathbb{S}^d$ that achieves the equality in the Welch bound [STDH07, CRT08]:

$$\max_{i \neq j} |x_i \cdot x_j| \geq \sqrt{\frac{N-d-1}{(d+1)(N-1)}}.$$

An ETF is called maximal, if it achieves equality in the Gerzon's bound:

$$\#\mathcal{C} \leqslant \frac{(d+1)(d+2)}{2}.$$

In effect, an ETF contains the largest possible number of points that maximize the minimal pairwise distance. The smallest dimension for which it is not known whether a maximal real ETF exists is $d = 118$ (so the corresponding dimension of the ambient space is 119) [BY13].

Goal 3. *Tabulate minimizers of the real p-frame potential on $\mathbb{S}^d$ for dimensions $d > 22$.*

On the other hand, it is the subject of the famous Zauner's conjecture that complex ETF (that is, ETFs in $\mathbb{S}^d$ in $\mathbb{C}^{d+1}$) exist for every dimension d. Such collections are known in quantum information theory as symmetric informationally-complete positive operator-valued measures (SIC-POVMs), and Zauner's conjecture will have important ramifications in this field [SG10, CKM16, ABFG19, FS]. Since it follows from Theorem 7 that complex ETF optimize the energy I_p for $2 < p < 4$, obtaining any results about them may be instrumental in proving Zauner's conjecture.

Conjecture 3.1 (Zauner)**.** *Complex minimizers of I_3 are ETFs.*

The above discussion concerns only the rather limited set of tight designs, see also Table 1. The next question is whether weaker results can be established for more general classes of kernels f; vice versa, whether specializing the kernel yields improved characterization of the minimizing measure. Indeed, we have a partial result for the case when f has finite number of positive coefficients in its expansion in terms of Gegenbauer polynomials. This should be viewed in contrast with the aforementioned fact that σ_d minimizers I_f if and only if f has all positive coefficients in the Gegenbauer expansion.

Theorem 8. *[BGM+19b] Suppose $\mathcal{N}_+, \mathcal{N}_- \subset \mathbb{N} \cup \{0\}$, such that $\#\mathcal{N}_+ < \infty$ and $\mathcal{N}_+ \cap \mathcal{N}_- = \emptyset$. Let*

$$f(t) := \sum_{i \in \mathcal{N}_+} a_i C_i(t) - \sum_{j \in \mathcal{N}_-} b_j C_j(t),$$

where $a_i, b_j \geq 0$, and C_n are the Gegenbauer polynomials. Then there exist minimizers of

$$I_f(\mu) = \iint_\Omega f(x \cdot y)\, d\mu(x) d\mu(y)$$

that are discrete.

Note that the p-frame kernel in a projective space has the form $\left(\frac{(t+1)}{2}\right)^{p/2}$. It has infinitely many positive, as well as negative Gegenbauer coefficients. The above theorem thus does not fully resolve the question of discreteness of the p-frame minimizers.

Goal 4. *Characterize the measure minimizing p-frame energies in the space $\mathcal{P}(\mathbb{S}^d)$. What assumptions on the kernel will guarantee that the minimizers are the extreme points of a certain convex set in $\mathcal{P}(\mathbb{S}^d)$?*

Conjecture 4.1. *Minimizers of a p-frame energy for $p \notin 2\mathbb{N}$ are discrete.*

Generalizing the last theorem to the case of infinite $\mathcal{N}_+$ will require understanding the structure of faces of the convex sets $S \subset \mathcal{P}(\mathbb{S}^d)$ of the form

$$S = \{\mu \in \mathcal{P}(\mathbb{S}^d) : \int f_i \, d\mu = c_i, \ i \in \mathcal{I}\}.$$

We shall finish this section by mentioning some partial progress towards the last conjecture.

Theorem 9 ([BGM+19a])**.** *Let $F(t) = |t|^p$, for $p > 0$ and $p \notin 2\mathbb{N}$. If μ is a minimizer of the p-frame energy I_F, then* $\operatorname{supp}(\mu)$ *has empty interior.*

Proposition 1 ([BGM+19a])**.** *Suppose F is a real-analytic, nonnegative function which is not positive definite on $\mathbb{S}^d$, and μ is a minimizer of I_F. Then* $\operatorname{supp}(\mu)$ *has empty interior.*

3.2 Multiple-precision optimization

To facilitate the studies of p-frames and magnetic anisotropy as described above, we propose to develop a multiple-precision optimization package by partially reimplementing the popular LBFGS optimization algorithm and combining it with the multiple precision C++ library, MPFR C++. The latter is a wrapper around the well-known MPFR library [FHL+07] developed by INRIA. Given the ill-conditioned nature of the problem of minimization of p-frame potential for large values of p, availability of such a package appears crucial for a number of experiments, for example, those related to the existence of equiangular tight frames.

To the best of our knowledge, there is no publicly available standalone package for multiple-precision optimization; alternative approaches include using an existing optimization algorithm in a language supporting arbitrary precision by design, such as *Julia* or *Mathematica*. This appears to be a less attractive path due to the overhead of the complex system, as well as due to the difficulty of embedding into other software.

Goal 5. *Implement a smooth multiple-precision optimization package based on LBFGS and MPFR. The implementation must be readily embeddable into other software.*

The PI has made partial progress towards producing such a package; a multiple-precision quasi-Newton optimizer based on Jorge Nocedal's LBFGS, and the aforementioned MPFR C++ library has been implemented [Vla19]. In its present state, the package handles unconstrained optimization only; weight and nonnegativity constraints are introduced by parametrization. For example, a nonnegative variable is represented by t^2, etc. In the future, PI plans to extend the applicability of this software by incorporating some of the features of the ROPTLIB library for optimization on Riemannian manifolds, developed by a group based, in particular, at FSU [HGAH17].

Goal 6. *Implement an extension of the above package for smooth multiple-precision optimization on manifolds, based on the ROPTLIB library.*

In high-dimensional optimization, it is important to sample the entire configurations space — which grows exponentially with dimension! To deal with the curse of dimensionality in medium-sized dimensions (10–40), we intend to implement a set of CUDA routines for parallel sampling of the phase space, using a Metropolis-type sampling procedure. The result of such sampling will be afterwards refined by the multiple precision package. One of the approaches we plan to experiment with, is using the so-called Lengevin dynamics, in which the interacting particles are equipped with mass, so that the interaction force changes their moments [CF19]. As an illustration of probabilistic sampling of the configuration, we shall cite the corresponding algorithm. Here $\wedge$ denotes taking minimum of two quantities; β_N is the "inverse temperature"

Algorithm 2: Metropolis adjusted Langevin algorithm [CF19]

for $k = 1, 2, \dots$ **do**

- K$\leftarrow$ Gaussian transition kernel associated to the Markov chain of the Euler discretization of the dynamics
- Draw a proposal $\tilde{x}_{k+1}$ according to the kernel $K(x_k, \cdot)$
- Compute the probability
$$p_k = 1 \wedge \frac{K(\tilde{x}_{k+1}, x_k) e^{-\beta_N H_N(\tilde{x}_{k+1})}}{K(x_k, \tilde{x}_{k+1}) e^{-\beta_N H_N(x_k)}},$$
- Set
$$x_{k+1} = \begin{cases} \tilde{x}_{k+1} & \text{with probability } p_k; \\ x_k & \text{with probability } 1 - p_k. \end{cases}$$

parameter; $H_N(x)$ is the potential created by the first N charges at the point x. Intuitively, the candidate point $\tilde{x}_{k+1}$ is accepted if it has sufficiently low energy.

It is not hard to see that the sampling performed in the algorithm can be made parallel, as different samples are completely independent. This makes it a natural candidate for execution on the GPU.

Goal 7. *Implement a random energy landscape sampler, executed on GPU.*

Since modern GPUs support only single/double machine precision, the output of such sampling will be further refined using a multiple-precision implementation on the CPU. In particular, it will be beneficial to implement distributed refinement of the output of Metropolis sampling, using multiple CPUs.

Goal 8. *Implement distributed refinement of the output of Metropolis sampling, using multiple CPUs. Similarly, perform sampling on multiple GPUs.*

4 Broader impact and outreach

As discussed above, minimization of p-frame potentials is related to compressed sensing, tight frames, and can give important insights into the existence of maximal ETFs. Numerical investigation of related energies can potentially be used to verify existence of certain strongly regular graphs (SRGs). More generally, a study of the minimizers of non-positive definite functionals can have important impact on the understanding of a number of physical models; as an example, the observation of dicreteness of the minimizers of such

functionals, although in a less general setting, has been made independently by a group studying causal variational principles [FS13].

An efficient optimization package supporting multiple-precision computations suggested above can be used to study a number of ill-conditioned problems, such as eigenvalues of large matrices, existence of high-dimensional combinatorial structures (SRGs, ETFs, etc). Study of the asymptotics of Riesz energies on fractal sets will require combining tools from geometric measure theory and ergodic theory; because fractals can be used as models of porous media, development of such tools may be very valuable for mathematical physics.

The project will result in publications relevant for the research groups based at University of Minnesota, University of Texas Rio Grande Valley, and Vanderbilt University, as well as abroad at University of Regensburg, Germany, University of Innsbruck and Graz University of Technology, Austria, and Imperial College London, UK. Researchers at the mentioned locations, as well as elsewhere, will benefit from the source code produced within the project, which will be released under an open source license.

The PI participates in the Analysis Seminar at Florida State University, and will participate in the organization of Analysis-related conferences at FSU. The PI is a co-organizer of a Special Section on "Frames, designs, and optimal spherical configurations" at JMM 2020. He will participate in a Collaborate@ICERM meeting in the Summer of 2020, dedicated to the ongoing research on the topic of this proposal.

The general outreach efforts conducted by the PI include participation in Math Fun Day at Florida State University, which is a major outreach activity of the Department of Mathematics, as well as the talks in the Undergraduate Math seminar, and the Math Circle at Vanderbilt University.

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