On the Search for Tight Frames of Low Coherence

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Abstract
We introduce a projective Riesz $s$-kernel for the unit sphere $S^{d-1}$ and investigate properties of $N$-point energy minimizing configurations for such a kernel. We show that these configurations, for $s$ and $N$ sufficiently large, form frames that are well-separated (have low coherence) and are nearly tight. Our results suggest an algorithm for computing well-separated tight frames which is illustrated with numerical examples.

Keywords Frame · Energy · Tight · Coherence · Separation

Mathematics Subject Classification Primary 42C15 · 31C20 · Secondary 42C40 · 74G65
1 Introduction

A set of vectors $X = \{x_i\}_{i \in I}$ is a frame for a separable Hilbert space $H$ if there exist $A, B > 0$ such that for every $x \in H$,

$$A \|x\|^2 \leq \sum_{i \in I} |\langle x, x_i \rangle|^2 \leq B \|x\|^2.$$  

The constant $A$ (resp. $B$) is called the lower (resp. upper) frame bound. When $A = B$, $X$ is called a tight frame, which generalizes the concept of an orthonormal basis in the sense that the recovery formula $x = \frac{1}{A} \sum_{i \in I} \langle x, x_i \rangle x_i$ holds for every $x \in H$. For the finite dimensional space $H = \mathbb{H}^d$, where $\mathbb{H} = \mathbb{R}$ or $\mathbb{C}$, $X = \{x_i\}_{i=1}^N$ is a frame of $\mathbb{H}^d$ if and only if $\{x_i\}_{i=1}^N$ spans $\mathbb{H}^d$. We shall also use $X$ to denote the matrix whose $i$th column is $x_i$ and therefore we have

$X$ is tight with frame bound $A \iff XX^* = A I_d$,

where $I_d$ is the $d \times d$ identity matrix.

Let $S(d, N) := \{X = \{x_i\}_{i=1}^N \subset \mathbb{H}^d : \|x_i\| = 1\}$ be the collection of all $N$-point configurations on $\mathbb{S}^{d-1}$, the unit sphere of $\mathbb{H}^d$, where $\| \cdot \|$ denotes the $\ell_2$ norm. If we have a unit norm tight frame $X \in S(d, N)$, then it is well known that the frame bound has to be $N/d$ since

$$XX^* = \frac{N}{d} I_d. \quad (1.1)$$

Benedetto and Fickus show in [2] that frames that attain

$$\min_{X \in S(d, N)} \sum_{i \neq j} |\langle x_i, x_j \rangle|^2 \quad (1.2)$$

are precisely the unit norm tight frames. We will call the function $|\langle x, y \rangle|^2$ the frame potential kernel. Ehler and Okoudjou [23] generalized this result to the $p$-frame potential kernel $|\langle x, y \rangle|^p$, see also [5] for recent results on $p$-frames.

Separation is a desirable property of a frame. It is quantified by the coherence $\xi(X)$ of a frame defined for $X \in S(d, N)$ by

$$\xi(X) := \max_{i \neq j} |\langle x_i, x_j \rangle|.$$

The smaller the coherence, the better separated the frame is.

A straightforward method to find well-separated frames is to solve

$$\xi_N := \min_{X \in S(d, N)} \xi(X) = \min_{X \in S(d, N)} \max_{i \neq j} |\langle x_i, x_j \rangle|, \quad (1.3)$$

\footnote{Depending on the context, we either consider $X$ to be a multiset, allowing for repetition, or as an ordered list.}

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which has been studied in several works including Welch [41], Conway et al. [20], Strohmer and Heath [39], and more recently [6, 26]. The problem (1.3) is often referred as the best line-packing problem because it asks how to arrange \( N \) lines in \( \mathbb{H}^d \) so that they are as far apart as possible. Conway et al. [20] made extensive computations on this problem from a more general perspective: how to best pack \( n \)-dimensional subspaces in \( \mathbb{R}^m \)? There are also many other contributions using tools in geometry and combinatorics [21], and statistics [1]. A minimizer of (1.3) is called a Grassmannian frame by [39] and we shall use this terminology as well.

Our goal in this paper is to develop methods for generating tight frames with low coherence using energy minimization on the projective space \( \mathbb{H}P^{d-1} \), which consists of all lines in \( \mathbb{H}^d \) through the origin; namely, sets of the form

\[
\ell(x) := \{\alpha x : \alpha \in \mathbb{H}\},
\]

for some \( x \in \mathbb{S}^{d-1} \). We endow \( \mathbb{H}P^{d-1} \) with the metric

\[
\rho(\ell(x), \ell(y)) := \sqrt{2 - 2|\langle x, y \rangle|^2}, \quad x, y \in \mathbb{S}^{d-1},
\]

which is the ‘chordal’ distance\(^2\) and utilize kernels on \( \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \) of the form:

\[
K(x, y) = f(\rho(\ell(x), \ell(y))) = f\left(\sqrt{2 - 2|\langle x, y \rangle|^2}\right), \quad x, y \in \mathbb{S}^{d-1} \subset \mathbb{H}^d.
\]

The energy of \( X = X_N = \{x_1, \ldots, x_N\} \) with respect to the kernel \( K \) is given by

\[
E_K(X_N) := \sum_{i \neq j} K(x_i, x_j).
\]

One seeks the infimum of (1.7) over all possible \( N \) point configurations on \( \mathbb{S}^{d-1} \). Assuming \( K \) is lower semi-continuous on \( \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \) so the infimum is attained, we define the \( N \)-point minimal energy of kernel \( K \) as

\[
\mathcal{E}_K(\mathbb{S}^{d-1}, N) := \min_{X \in \mathcal{S}(d, N)} E_K(X).
\]

An \( N \)-point configuration that achieves the minimum (1.8) will be denoted by \( X_N^*(K, \mathbb{S}^{d-1}) \) (or \( X_N^* \), when there is no ambiguity). So far the minimal energy and optimal configuration have been confined to the sphere and generalizes to any compact set \( A \), and will be denoted as \( \mathcal{E}_K(A, N), X_N^*(K, A) \) respectively. Note that the frame potential \( |\langle x, y \rangle|^2 \) is of the form (1.6) and that the energy minimizers are precisely the unit norm tight frames. However, in general for \( N > d \), these minimizers may not consist of well-separated lines.

To achieve well separation of lines our approach is to first consider a class of kernels that are strongly repulsive and analyze the approximate tightness of their

\(^2\) The chordal distance between the lines \( \ell(x) \) and \( \ell(y) \) is given by \( \min\{\|x - uy\| : u \in \mathbb{H}, |u| = 1\} \).
energy minimizers relative to their frame potential energy. Specifically, we introduce the \textit{Riesz projective s-kernel}

\[
G_s(x, y) := \begin{cases} 
\log \frac{1}{1 - |\langle x, y \rangle|^2}, & s = 0 \\
\frac{1}{(1 - |\langle x, y \rangle|^2)^{s/2}}, & s > 0
\end{cases}
\]  

(1.9)

for \(x, y \in \mathbb{S}^{d-1}\) and seek solutions to the problem

\[
\min_{X \in S(d, N)} \sum_{i \neq j} G_s(x_i, x_j).
\]  

(1.10)

The kernel \(G_s\) is a modification of the classical \textit{Riesz s-kernel} defined for \(x, y\) in a normed linear space \((V, \| \cdot \|)\) as

\[
R_s(x, y) := \begin{cases} 
\log \frac{1}{\|x - y\|}, & s = 0 \\
\frac{1}{\|x - y\|^s}, & s > 0
\end{cases}
\]  

(1.11)

In fact, as we will show in (3.5), the projective Riesz \(s\)-kernel \(G_s\) can also be represented in terms of \(R_s\) for an appropriate subspace \(V\) of matrices with the Frobenius norm.

Notice that minimizers of (1.10) will avoid antipodal points since the energy in that case would be infinite. The connection between projective Riesz \(s\)-kernels and Riesz \(s\)-kernels is more immediate in the real case \(\mathbb{R}^d\); since \(\|x \pm y\|^2 = 2 \pm 2\langle x, y \rangle\), we have

\[
\frac{1}{(1 - |\langle x, y \rangle|^2)^{s/2}} = \frac{2^s}{\|x - y\|^s \|x + y\|^s}.
\]

Thus the projective Riesz kernel is just the Riesz kernel with the multiplicative factor \(\|x + y\|^s\) to account for antipodal points.

A major focus of this paper is to exploit connections between \(G_s\) and \(R_s\) and reduce solving the projective Riesz \(s\)-kernel minimization problem (1.10) to solving

\[
\min_{X \subset D, |X| = N} \sum_{i \neq j} R_s(x_i, x_j),
\]  

(1.12)

where we take \(D\) to be the projective space, but embedded in a higher dimensional real vector space (see Sect. 3.2). There are well established theorems available in the minimal energy literature for Riesz \(s\)-kernels (see e.g. [8]) and we shall review some of them in Sect. 2.

The projective Riesz \(s\)-kernel for \(s < 0\) defined by \(G_s(x, y) := -(1 - |\langle x, y \rangle|^2)^{-s/2}\) is also interesting. For such \(s\) we will be solving

\[
\min_{X \in S(d, N)} \sum_{i \neq j} -(1 - |\langle x, y \rangle|^2)^{-s/2} \quad (s < 0).
\]  

(1.13)
This coincides with (1.2) when \( s = -2 \). This paper shall focus on the \( s \geq 0 \) case in the analysis, but our numerical experiments will include optimal configurations of (1.13).

The contributions of this paper are two-fold:

- Derive minimal energy results for the projective Riesz kernel. See Theorems 4.1, 5.1, and 5.4.
- Develop methods for constructing nearly tight and well-separated frames. See Theorems 6.3 and 6.4 and numerical results in Sect. 7.3.

2 Minimal Energy Background

In this section we will introduce some necessary background on minimizing discrete energy and its relation to the continuous energy.

The discrete minimal energy problem is known to be challenging, and we have very limited knowledge about the optimal configuration even for the classical Riesz kernel case (1.12) on the 2-dimensional sphere. The following theorem settles the case when points are on a circle of a real vector space for a large class of kernels that includes Riesz kernels.

**Theorem 2.1** (Fejes-Tóth [24]) If \( r > 0 \) and \( f : (0, 2r] \to \mathbb{R} \) is a non-increasing convex function defined at 0 by the (possibly infinite) value \( \lim_{t \to 0^+} f(t) \), then any \( N \) equally spaced points on a circle of radius \( r \) (in \( \mathbb{R}^m \)) minimizes the discrete energy \( E_K(X_N) \) for the kernel \( K(x, y) = f(||x - y||) \). If in addition, \( f \) is strictly convex, then no other \( N \)-point configuration on this circle is optimal.

Less is known regarding optimal configurations for (1.12) beyond \( S^1 \). For optimality of configurations with particular cardinality \( N \) and dimension \( d > 1 \), see [18] and [8]. On the other hand, many asymptotic results (as \( N \to \infty \)) for optimal configurations on the sphere as well as on \( \mathbb{R}^d \) are known (for examples of recent results, see [4], [31]).

For a set of \( N \) points \( X = \{x_i\}_{i=1}^N \), the separation distance of \( X \) is defined as

\[
\delta(X) := \min_{i \neq j} \|x_i - x_j\|.
\]

The best-packing problem is to find the \( N \)-point configuration on \( A \) that maximizes the separation distance:

\[
\delta_N(A) = \max_{X \subset A, |X|=N} \delta(X) = \max_{X \subset A, |X|=N} \min_{i \neq j} \|x_i - x_j\|. \tag{2.1}
\]

It is immediate, for example, that the best \( N \)-point packing of \( S^1 \subset \mathbb{R}^2 \) consists of \( N \) equally spaced points on the circle.

When \( s \to \infty \), the minimization problem with respect to the Riesz kernel \( R_s(x, y) \)

\[
\min_{X \subset A, |X|=N} E_{R_s}(X)
\]
turns into the best-packing problem (2.1); more precisely,

**Theorem 2.2** [8] If \( N \geq 2 \) and \( A \subset \mathbb{R}^m \) is a compact set of cardinality at least \( N \), then

\[
\lim_{s \to \infty} \mathcal{E}_{R_s}(A, N)^{1/s} = 1/\delta_N(A),
\]

where \( R_s \) is the Riesz kernel defined in (1.11). Furthermore, if \( X_s \) is an optimal configuration that achieves \( \mathcal{E}_{R_s}(A, N) \), then every cluster point as \( s \to \infty \) of the set \( \{X_s\}_{s>0} \) on \( A \) is an \( N \)-point best-packing configuration on \( A \).

This discrete minimal energy problem is related to a continuous energy problem as we next describe. Let \( \mathcal{M}(A) \) be the set of probability measures supported on \( A \). For a general kernel \( K \), the potential function of a measure \( \mu \in \mathcal{M}(A) \) with respect to \( K \) is defined as

\[
U_K^\mu(x) := \int_A K(x, y) \, d\mu(y),
\]

provided the integral exists as an extended real number. The energy of \( \mu \) is defined as

\[
I_K(\mu) := \int_A U_K^\mu(x) \, d\mu(x) = \iint_{A \times A} K(x, y) \, d\mu(x)d\mu(y),
\]

and the Wiener constant is

\[
W_K(A) := \inf_{\mu \in \mathcal{M}(A)} I_K(\mu). \tag{2.2}
\]

Likewise this infimum can be achieved, and the probability measure that optimizes the above problem is called the \( K \)-equilibrium measure. The \( K \)-capacity of the set \( A \) is defined by

\[
\text{cap}_K(A) := \frac{1}{W_K(A)}.
\]

A set \( A \) has zero capacity means that \( W_K(A) = \infty \), which makes the problem (2.2) trivial since every probability measure generates \( \infty \) energy.

We now present a classical theorem connecting the discrete minimal energy problem to the continuous one. Before that we introduce the weak* limit of measures. A sequence of measures \( \mu_n \) converges weak* to \( \mu \) if for every continuous function \( f \) on \( A \),

\[
\lim_{n \to \infty} \int f \, d\mu_n = \int f \, d\mu.
\]
We also define $\delta_x$ to be the point mass probability measure on the point $x$. Moreover, given a finite collection of points $X$, its normalized counting measure is defined as

$$\nu(X) = \frac{1}{|X|} \sum_{x \in X} \delta_x.$$  

**Theorem 2.3** ([17], [8, Theorem 4.2.2]) If $K$ is a lower semicontinuous and symmetric kernel on $A \times A$, where $A \subset \mathbb{R}^m$ is an infinite compact set, then

$$\lim_{N \to \infty} \frac{E_K(A, N)}{N^2} = W_K(A).$$  

Moreover, every weak* limit measure (as $N \to \infty$) of the sequence of normalized counting measures $\nu(X^*_N)$ is a $K$-equilibrium measure.

The proof of Theorem 2.3 for the case of a Riesz kernel can also be found in the book by Landkof [34, Eq. (2.3.4)].

We now review two important facts concerning Riesz kernels.

**Theorem 2.4** [7,8,37] Let $A \subset \mathbb{R}^m$ be a compact infinite subset of an $\alpha$-dimensional $C^1$-manifold with $A$ of positive $\alpha$-dimensional Hausdorff measure.

1. If $s \in (0, \alpha)$, then the $R_s$-equilibrium measure on $A$ is unique. Moreover, if the potential function $U_{R_s}^\mu$ is constant on $A$, then $\mu$ is the $R_s$-equilibrium measure on $A$.

2. If $s \in [\alpha, \infty)$, then $A$ has $R_s$-capacity zero. Moreover, if $X^*_N(R_s, A)$ denotes an $R_s$-energy optimal $N$-point configuration for $N \geq 2$, then the sequence of normalized counting measures $\nu(X^*_N(R_s, A))$ converges to the uniform measure (normalized Hausdorff measure) on $A$ in the weak* sense as $N \to \infty$ (this is a special case of the so-called Poppy-seed bagel theorem).

### 3 An Overview of the Problem on the Sphere

#### 3.1 Projectively Equivalent Configurations

Note that for a kernel $K$ of the form (1.6), the energy $E_K(X)$, $X = \{x_i\}_{i=1}^N \in S(d, N)$, is invariant under any of the following operations on $X$:

(i) Apply a unitary operator (or orthogonal operator if $\mathbb{H} = \mathbb{R}$) on $X$ as $\{Ux_i\}_{i=1}^N$;
(ii) Change the sign of any $x_i$;
(iii) Permute $x_1, \ldots, x_N$.

Any configuration $Y$ obtained from $X$ by applying these operations is said to be projectively equivalent to $X$. For example, $\{x_1, x_2, x_3, x_4\}$ is projectively equivalent to $\{Ux_4, Ux_2, -Ux_3, Ux_1\}$. 

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Theorem 5.1 below states that the configuration of equally spaced points on the half-circle,
\[ X_N^{(h)} := \{ e^{i\theta}, e^{i\frac{\pi}{N}}, e^{i\frac{2\pi}{N}}, \ldots, e^{i\frac{(N-1)\pi}{N}} \} \subset \mathbb{R}^2, \] (3.2)
is optimal for (1.8) for a certain class of kernels \( K \).

### 3.2 From Sphere to the Projective Space

The projective space \( \mathbb{HP}^{d-1} \) can be embedded isometrically into the space of \( d \times d \) Hermitian matrices, denoted by \( \mathbb{HM}^h_{d \times d} \) as we next describe. Note that \( \mathbb{HM}^h_{d \times d} \) is a real vector space for both \( \mathbb{H} = \mathbb{R} \) and \( \mathbb{H} = \mathbb{C} \) with inner product in \( \mathbb{HM}^h_{d \times d} \) defined as \( \langle M_1, M_2 \rangle = \text{Trace}(M_1^* M_2) \). This inner product induces the Frobenius norm \( \| M \| = \| M \|_F \) on \( \mathbb{HM}^h_{d \times d} \). We further note that \( \mathbb{HM}^h_{d \times d} \) with the Frobenius norm can be identified with the Euclidean space \( \mathbb{R}^m \) where \( m = (d^2 + d)/2 \) when \( \mathbb{H} = \mathbb{R} \) and \( m = d^2 \) when \( \mathbb{H} = \mathbb{C} \) (e.g., when \( \mathbb{H} = \mathbb{R} \) and \( M = (M_{i,j}) \) we take any ordering of the \( m \) numbers \( \sqrt{2} M_{i,j} \) for \( i < j \) and \( M_{i,j} \) for \( i = j \)).

Recalling (1.4), we define \( \Psi : \mathbb{HP}^{d-1} \to \mathbb{HM}^h_{d \times d} \) as \( \Psi(\ell(x)) := px \) with \( px := \chi y^*x \) and \( x \in S^{d-1} \). Clearly, \( \Psi \) is well defined (i.e., independent of the choice of the representative of the line). We denote the range of \( \Psi \) by \( \mathcal{D} \); that is, \( \mathcal{D} := \Psi(\mathbb{HP}^{d-1}) = \Phi(S^{d-1}) \) where \( \Phi := \Psi \circ \ell \).

For \( x, y \in S^{d-1} \), the following well known equality (see, e.g. \cite{19}) establishes that \( \Psi \) is an isometry:
\[ \rho(\ell(x), \ell(y))^2 = 2 - 2|\langle x, y \rangle|^2 = \| px - py \|_F^2 \]
\[ = \| \Phi(x) - \Phi(y) \|_F^2. \] (3.3)

It is used, for example, in works on phase retrieval, see e.g. \cite{13, 28}. For the reader’s convenience we note that the middle equality in (3.3) follows using the cyclic property of the trace:
\[ \| px - py \|_F^2 = 2 - \langle px, py \rangle - \langle py, px \rangle \]
\[ = 2 - \text{Trace}(y^*xx^*y) - \text{Trace}(x^*yy^*x) = 2 - 2|\langle x, y \rangle|^2, \]
from which we also get
\[ \langle px, py \rangle = |\langle x, y \rangle|^2. \] (3.4)

Note that (3.3) shows that \( \Psi \) is an isometric embedding of \( \mathbb{HP}^{d-1} \) in \( \mathbb{HM}^h_{d \times d} \), and so we identify \( \mathbb{HP}^{d-1} \) with \( \mathcal{D} \). We remark that \( \mathcal{D} \) is a real analytic manifold whose dimension \( \dim(\mathcal{D}) = \dim(\mathbb{HP}^{d-1}) \) is \( d - 1 \) in the case \( \mathbb{H} = \mathbb{R} \) and \( 2d - 2 \) in the case \( \mathbb{H} = \mathbb{C} \) (see \cite{6} or \cite{35}).

Now we are able to consider a kernel of the form \( K(x, y) = f(\sqrt{2 - 2|\langle x, y \rangle|^2}) \) on \( S^{d-1} \times S^{d-1} \) as a kernel \( \tilde{K}(px, py) = f(\| px - py \|) \) on \( \mathcal{D} \times \mathcal{D} \).
Specifically the projective Riesz $s$-kernel (see (1.9)) can be reexpressed as

$$
G_s(x, y) = \begin{cases} 
\log \frac{2}{\|p_x - p_y\|_{F}^2} = \log 2 + 2 R_s(p_x, p_y), & s = 0 \\
\frac{2^{s/2}}{2^{s/2} \|p_x - p_y\|_{F}^2} = 2^{s/2} R_s(p_x, p_y), & s > 0.
\end{cases}
$$

(3.5)

This allows us to reformulate the minimal projective energy problem in terms of the Riesz minimal energy problem on the set $D$. This technique was also employed in [15]. In the next two sections we apply results of Sect. 2 for the problems

$$
\min_{\mu \in \mathcal{M}(D)} I_{R_s}(\mu) \quad (3.6)
$$

$$
\min_{\{p_i\}_{i=1}^N \subset D} \sum_{i \neq j} R_s(p_i, p_j). \quad (3.7)
$$

Similarly, the Grassmannian problem (1.3) is equivalent to the best-packing problem (2.1) on the projective space, which is to maximize the smallest pairwise distance between all the lines (frame vectors). Let $P = \{p_i\}_{i=1}^N \subset D$. For any point $p_i \in D$, we can find $x_i \in \mathbb{S}^{d-1}$ such that $p_i = x_i x_i^*$. By (3.3),

$$
\delta^2(P) = \min_{i \neq j} \|p_i - p_j\|^2 = \min_{i \neq j} (2 - 2|\langle x_i, x_j \rangle|) = 2 - 2 \max_{i \neq j} |\langle x_i, x_j \rangle| = 2 - 2 \xi(X). \quad (3.8)
$$

So

$$
\delta_N^2(D) = \max_{\{x_i\}_{i=1}^N \subset \mathbb{S}^{d-1}} \delta^2(P) = \max_{\{x_i\}_{i=1}^N \subset \mathbb{S}^{d-1}} (2 - 2 \xi(X)) = 2 - 2 \xi_N. \quad (3.9)
$$

The last equality is from the definition (1.3).

For any Borel probability measure $\mu$ on the sphere, this embedding also induces the pushforward (probability) measure $\mu_{\text{proj}}$ on $D \subset \mathbb{H}^{d \times d}$. By definition of a pushforward measure,

$$
\mu_{\text{proj}}(B) := \mu(\Phi^{-1}(B)), \quad \text{for Borel measurable } B \subset D. \quad (3.10)
$$

We shall also write $\Phi(\mu)$ for $\mu_{\text{proj}}$.

To better understand $\mu_{\text{proj}}$, we further consider the symmetrization $\mu_{\text{sym}}$ of a measure $\mu \in \mathcal{M}(\mathbb{S}^{d-1})$ defined as

$$
\mu_{\text{sym}}(B) = \begin{cases} 
\frac{\mu(B) + \mu(-B)}{2}, & \mathbb{H} = \mathbb{R} \\
\frac{1}{2\pi} \int_0^{2\pi} \mu(e^{i\theta} B) d\theta, & \mathbb{H} = \mathbb{C},
\end{cases}
$$

(3.11)

for Borel measurable $B \subset \mathbb{S}^{d-1}$. 

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It is not difficult to show that \( \mu_{\text{sym}} = \tilde{\mu}_{\text{sym}} \) if and only if the pullback measures \( \mu \circ \ell^{-1} \) and \( \tilde{\mu} \circ \ell^{-1} \) agree. The injectivity of \( \Psi \) then shows

\[
\Phi(\mu) = \Phi(\tilde{\mu}) \iff \mu_{\text{sym}} = \tilde{\mu}_{\text{sym}}.
\]  

(3.12)

Let \( \sigma_{d-1} \) be the uniform measure (normalized surface measure) on \( S^{d-1} \). Then \( \Phi(\sigma_{d-1}) \), the pushforward measure of \( \sigma_{d-1} \) under \( \Phi \), is the uniform measure on \( D \). In fact, \( \Phi(\sigma_{d-1}) \) is the Haar invariant measure induced by the unitary group (see [15, Sect. 4.2]).

4 Large N Behavior of Optimal Configurations

We first focus on the continuous problem

\[
\min_{\mu \in \mathcal{M}(S^{d-1})} \int_{S^{d-1} \times S^{d-1}} G_s(x, y) \, d\mu(x) d\mu(y),
\]  

(4.1)

The results are of independent interest, and will be used in Sect. 6.

For future reference, we set

\[
I_s(\mu) := I_{Rs}(\mu) = \int_{D \times D} R_s(x, y) \, d\mu(x) d\mu(y)
\]

and

\[
J_s(\mu) := I_{Gs}(\mu) = \int_{S^{d-1} \times S^{d-1}} G_s(x, y) \, d\mu(x) d\mu(y).
\]

As previously discussed, the projective space \( D \) embedded in \( \mathbb{R}^m \) is a smooth \((C^\infty)\) compact manifold, so Theorem 2.4 applies with \( A = D \) and \( \alpha = \dim(D) \).

Theorem 4.1 For the projective Riesz kernel \( G_s(x, y) \), the following properties hold.

1. If \( 0 \leq s < \dim(D) \), then \( \mu \) is a \( G_s \)-equilibrium measure on \( S^{d-1} \) if and only if its symmetrized measure \( \mu_{\text{sym}} \) is the normalized surface measure \( \sigma_{d-1} \) on \( S^{d-1} \).
2. If \( s \geq \dim(D) \), then \( S^{d-1} \) has \( G_s \)-capacity 0.
3. Let \( s \geq 0 \) and let \( X_N^* \) be a \( G_s \)-optimal \( N \)-point configuration on \( S^{d-1} \) for \( N \geq 2 \). Then the sequence of normalized counting measures \( \nu(\Phi(X_N^*)) \) converges weak* to the uniform measure \( \Phi(\sigma_{d-1}) \) on \( D \) as \( N \to \infty \).

Proof (1) When \( s > 0 \), by (3.5) and the definition of a pushforward measure,

\[
U_{Gs}^{\mu}(x) = \int_{S^{d-1}} G_s(x, y) \, d\mu(y) = \int_{D} \frac{2^{2/s}}{\| p_x - p \|^s} d\mu_{\text{proj}}(p) = \text{const} \cdot U_{Rs}^{\mu_{\text{proj}}}(p_x).
\]  

(4.2)

A similar equality holds for the log case \( s = 0 \): \( U_{Gs}^{\mu}(x) = \text{const} \cdot U_{Rs}^{\mu_{\text{proj}}}(p_x) + \text{const} \).
Thus for $s \geq 0$, the uniform measure $\sigma_{d-1}$ produces a constant potential function with the kernel $G_s$, so $\Phi(\sigma_{d-1})$ also produces a constant potential function with the Riesz kernel $R_s$. By Theorem 2.4(1), $\Phi(\sigma_{d-1})$ must be the unique minimizer of (3.6).

On the other hand, similar to (4.2), $J_\gamma(\mu) = \int_{S^{d-1}} \int_{S^{d-1}} G_s(x, y) \, d\mu(x) d\mu(y) = \int_D \int_D \frac{2^{2/s}}{\|p - p'\|^s} \, d\mu_{\text{proj}}(p) d\mu_{\text{proj}}(p') = \text{const} \cdot I_s(\mu_{\text{proj}}).$ (4.3)

Again a similar equality holds for the log case. This implies that $\mu$ is a minimizer of (4.1) if and only if $\Phi(\mu) = \mu_{\text{proj}}$ is a minimizer of (3.6), which has to be $\Phi(\sigma_{d-1})$. By (3.12), this is equivalent to $\mu_{\text{sym}} = (\sigma_{d-1})_{\text{sym}} = \sigma_{d-1}$. This proves that $\mu$ is an equilibrium measure if and only if its symmetrized measure $\mu_{\text{sym}}$ is $\sigma_{d-1}$.

(2) With the relation (4.3), this is a direct consequence of Theorem 2.4(2).

(3) For the discrete case, similar to (4.3), we have $E_{G_s}(X_N) = \text{const} \cdot E_{R_s}(\Phi(X_N)) + \text{const}$. So $X_N^\ast$ be a $G_s$-optimal $N$-point configuration on $S^{d-1}$ if and only if $\Phi(X_N^\ast)$ is an optimal configuration for the Riesz kernel $R_s$ on $D$.

By Theorem 2.3, we conclude that the normalized counting measure $\nu(\Phi(X_N^\ast))$ converges to the $R_s$-equilibrium measure on $D$ in the weak* sense. As shown in part (1), this unique equilibrium measure is $\Phi(\sigma_{d-1})$, when $s \in [0, \dim(D))$. When $s \geq \dim(D)$, by Theorem 2.4(2), we also have $\nu(\Phi(X_N^\ast))$ converges to $\Phi(\sigma_{d-1})$. \qed

5 Discrete Minimal Energy Problem

In this section we consider discrete extremal energy problems, for a general class of projective kernels of the form (1.6). Once again, the optimal configuration is an equivalent class in the sense of (3.1). Theorem 5.1 is for the 1-dimensional sphere in the real vector space while Theorem 5.4 is a general result over $\mathbb{H}$. Corollary 5.6 addresses the special projective Riesz kernel case (1.10).

Theorem 5.1 If $f : (0, \sqrt{2}] \to \mathbb{R}$ is a non-increasing convex function defined at zero by the (possibly infinite) value $\lim_{t \to 0^+} f(t)$, then $X_N^{(h)}$ given in (3.2) is an optimal configuration on $\mathbb{R}P^1$ for the problem (1.8) where $K$ is as in (1.6). If, in addition, $f$ is strictly convex, then up to the equivalence relation in (3.1), no other $N$-point configuration is optimal.

Proof By (3.3), $K(x, y) = f(\|p_x - p_y\|)$, so we need to consider the minimal energy problem (1.8) with the kernel function to be $f(\|x - y\|)$ on the compact set $D = \Phi(S^1)$. The map $\Phi : S^1 \to \mathbb{R}M_{2 \times 2}^h$ is precisely $\Phi : (x, y) \to \begin{bmatrix} x^2 & xy \\ xy & y^2 \end{bmatrix}$. 

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As mentioned at the beginning of Sect. 3.2, $\mathbb{R}^{2 \times 2}_h$ is identified with $\mathbb{R}^3$ using the mapping
$$
\begin{bmatrix}
x^2 & xy \\
xy & y^2
\end{bmatrix} \rightarrow (x^2, \sqrt{2}xy, y^2).
$$
This way, $\mathcal{D}$ is a circle in $\mathbb{R}^3$ with radius $1/\sqrt{2}$.

With $r = 1/\sqrt{2}$, the function $f$ satisfies the assumptions of Theorem 2.1, so
$$
\sum_{i \neq j} K(x_i, x_j) = \sum_{i \neq j} f(\|p_{x_i} - p_{x_j}\|)
$$
is minimized if $p_{x_1}, p_{x_2}, \ldots, p_{x_N}$ are equally spaced on the circle $\mathcal{D}$. One can easily show that $\Phi$ maps equally spaced points on half $\mathbb{S}^1$ to equally spaced points on $\mathcal{D}$. So minimizers of (1.8) are precisely the equivalence class of equally spaced points on half of $\mathbb{S}^1$. \hfill \Box

\textbf{Remark 5.2} It is well known that $\mathbb{RP}^{d-1}$ is a compact Riemannian manifold. However, $\mathbb{RP}^{d-1}$ is topologically equivalent to a sphere only when $d = 2$.

\textbf{Remark 5.3} The frame potential kernel $|\langle x, y \rangle|^2$ can be written as $g(\sqrt{2} - 2|\langle x, y \rangle|^2)$, where $g(t) = 1 - t^2/2$ is not convex on $[0, \sqrt{2}]$. As a consequence, Theorem 5.1 cannot be applied to the frame potential kernel. The conclusion of Theorem 5.1 is however true, but there is no uniqueness (see [2]).

The discrete minimal energy problem for the Riesz $s$-kernel is in general very hard as mentioned previously. The situation is slightly better for kernels that are a function of absolute value of inner product, as we have the following general characterization when an equiangular tight frame (ETF) exists. A frame $X = \{x_i\}_{i=1}^N$ is equiangular if $|\langle x_i, x_j \rangle|/\|x_i\|\|x_j\|$ is a constant for all $i \neq j$. An ETF is a frame that is equiangular and tight. For frames in $\mathcal{S}(d, N)$, a necessary condition for the existence of ETF is $N \leq d(d + 1)/2$ for $\mathbb{H} = \mathbb{R}$ and $N \leq d^2$ for $\mathbb{H} = \mathbb{C}$. The coherence has the famous Welch bound
$$
\xi(X) \geq \sqrt{\frac{N - d}{d(N - 1)}}, \quad \text{for all } X \in \mathcal{S}(d, N),
$$
and is achieved by ETFs. This can be easily derived from the relation (cf. [19])
$$
N + N(N - 1)\xi(X)^2 \geq \sum_{i,j=1}^N |\langle x_i, x_j \rangle|^2
= \|XX^* - N/d I_d\|_F^2 + \frac{N^2}{d} \geq \frac{N^2}{d}.
$$
The Welch bound also coincides with the simplex bound of the chordal distance in [20]. We refer interested readers to [40] for more details and [25] for a table on existing ETFs. The second inequality in (5.2) also shows that the frame potential is minimized when the frame is tight.

The second theorem is for both the real and complex case.
Theorem 5.4  Let \( \tilde{f} : (0, 2] \to \mathbb{R} \) be a strictly convex and decreasing function defined at \( t = 0 \) by the (possibly infinite) value \( \lim_{t \to 0^+} \tilde{f}(t) \), and \( f : (0, \sqrt{2}] \to \mathbb{R} \) be a strictly convex and decreasing function defined at \( t = 0 \) by the (possibly infinite) value \( \lim_{t \to 0^+} f(t) \). If \( N \) and \( d \) are such that an ETF exists, then

(i) it is the unique optimal configuration of (1.8) for the kernel \( \tilde{K}(x, y) = \tilde{f}(2 - 2\|(x, y)\|^2) \);

(ii) it is also the unique optimal configuration of (1.8) for the kernel \( K(x, y) = f(\sqrt{2} - 2\|(x, y)\|^2) \).

Proof (i) From (3.3), \( \tilde{K}(x, y) = \tilde{f}(\|p_x - p_y\|^2) \). Let \( X = \{x_1, x_2, \ldots, x_N\} \) be an arbitrary configuration on the sphere and set \( P_i := p_{x_i} = x_i x_i^* \). Then, by (3.4),

\[
J := \sum_{i \neq j} \|P_i - P_j\|^2 = \sum_{i=1}^{N} \sum_{j \neq i} (2 - 2(P_i, P_j)) = \sum_{i=1}^{N} \left( 2(N - 1) - 2 \sum_{j=1}^{N} (P_i, P_j) + 2 \right)
\]

\[
= 2N^2 - 2 \sum_{i,j=1}^{N} |\langle x_i, x_j \rangle|^2 \leq 2N^2 - 2N^2/d,
\]

where the last inequality follows from (5.2). Thus,

\[
E_{\tilde{K}}(X) = \frac{N(N - 1)}{1} \cdot \frac{1}{N(N - 1)} \sum_{i \neq j} \tilde{f}(\|P_i - P_j\|^2)
\geq \frac{N(N - 1)}{1} \tilde{f} \left( \sum_{i \neq j} \frac{1}{N(N - 1)} \|P_i - P_j\|^2 \right)
= N(N - 1) \tilde{f} \left( \frac{J}{N(N - 1)} \right)
\geq N(N - 1) \tilde{f} \left( \frac{2N^2 - 2N^2/d}{N(N - 1)} \right)
= N(N - 1) \tilde{f} \left( \frac{2N(1 - 1/d)}{N - 1} \right). \tag{5.3}
\]

The first inequality becomes equality if and only if \( |\langle x_i, x_j \rangle| \) is constant for \( i \neq j \); i.e., \( X \) is equiangular. The second inequality becomes equality if and only if \( X \) is a unit norm tight frame. Therefore, if an ETF exists for a given \( d \) and \( N \), then this ETF is the unique \( \tilde{K} \)-energy minimizer.

Part (ii) is a direct consequence of (i). Indeed, \( f(\sqrt{2} - 2\|(x, y)\|^2) = g(2 - 2\|(x, y)\|^2) \), where \( g(t) = f(\sqrt{t}) \). Since \( f \) is decreasing and convex, the same holds for \( g \), to which we apply (i). \( \square \)
Remark 5.5 Theorem 5.4 shows that an ETF is universally optimal (see [18,19]) in the sense that it minimizes the energy for any potential that is a completely monotone function of distance squared in the projective space.

The assumption of Theorem 5.4 (part (i)) is weaker than that of Theorem 5.1 as reflected in the above proof. For example, Theorem 5.4 part (i) recovers Proposition 3.1 of [23] since \(|\langle x, y \rangle|_p^p = f(1 - |\langle x, y \rangle|^2)\) with \(f(t) = (1 - t)^{p/2}\). It is easy to verify that \(f(t)\) is decreasing and convex on \([0, 1]\) when \(p > 2\). However \((1 - t^2)^{p/2}\) is not convex, and therefore part (ii) cannot be used to recover Proposition 3.1 of [23]. We refer the interested reader to [16] for more results on \(p\)-frame potential.

Both Theorems 5.1 and 5.4 apply to the projective Riesz kernel since \(\log 1/t\) and \(1/\sqrt{t}\) are strictly decreasing and strictly convex.

Corollary 5.6 For the projective Riesz s-kernel minimization problem (1.10) when \(s \in [0, \infty)\),

(i) the configuration \(X_N^{(h)}\) defined in (3.2) is optimal for \(S^1 \subset \mathbb{R}^2\);
(ii) if it exists, an ETF is the optimal configuration for \(S^{d-1} \subset \mathbb{H}^d\).

Remark 5.7 The conclusions of Corollary 5.6 hold for \(s = \infty\) (best line-packing problem). These results were mentioned in [39] and are also implied by Theorem 6.1.

In particular, the optimal configuration of \(N = d + 1\) points that solves (1.10) is given by the vertices of a regular \(d\)-simplex because it is an ETF. When \(d = 3\), the results for ETF are well known for small values of \(N\). We summarize these results in Table 1, where we also compare the optimal configurations of the projective Riesz kernel and the classical Riesz kernel. They only share the same optimal configuration for the \(N = d + 1\) case. Moreover, ETFs are optimal configurations for the projective kernel while nothing is known for the Riesz kernel in general.

We have explained intuitively why the projective Riesz kernels are better at promoting well-separated frames than the Riesz kernel. This is reflected in Table 1. For the first case \(S^1\) when \(N = 4\), the optimal configuration for the projective Riesz kernel is two orthonormal bases with a 45 degree angle, which is a well-separated tight frame, while the optimal configuration for the Riesz kernel consists of 4 equally spaced points on \(S^1\). For the third row, an orthonormal basis is the optimal frame whereas 3 points on one great circle is not even a frame. For 6 points on a sphere, the Riesz optimal configuration is again two copies of the same orthonormal bases. More numerical support can be found in Sect. 7.

The Grassmannian frame consisting of 5 vectors is constructed by removing an arbitrary element of the optimal Grassmannian frame consisting of 6 vectors (ETF). The coherence of the Grassmannian frame (in both \(N = 5\) and \(N = 6\)) is \(1/\sqrt{5}\). We refer to [20] for more details.

It is not possible for 5 points to be an ETF in \(\mathbb{R}^3\), and the optimal configuration of (1.10) remains open to the best knowledge of the authors. The numerical experiments in Table 2 indicate that optimal configurations have exactly 2 distinct inner products. These inner products depend on the value \(s\). As \(s \rightarrow \infty\), Theorem 6.1 below implies that the inner products converge to \(1/\sqrt{5}\).
Table 1 Optimal configuration comparison on $\mathbb{S}^{d-1} \subset \mathbb{R}^d$

| proj. Riesz kernel $s \in [0, \infty)$ | Best line-packing $s = \infty$ | Riesz kernel $s \in [0, \infty)$ |
|----------------------------------------|-------------------------------|----------------------------------|
| $\mathbb{S}^1$, any $N$                | Equally spaced points on half circle | Equally spaced points on $\mathbb{S}^1$ |
| $\mathbb{S}^2$, $N = 2$               | Two orthogonal points          | Two antipodal points             |
| $\mathbb{S}^2$, $N = 3$               | Any orthonormal basis          | Vertices of an equilateral triangle on a great circle |
| $\mathbb{S}^2$, $N = 4$               | Vertices of a regular tetrahedron (simplex) |                                  |
| $\mathbb{S}^2$, $N = 5$               | Open, see Table 2              | Removing any vector from the $3 \times 6$ ETF, see [3,20] |
| $\mathbb{S}^2$, $N = 6$               | $3 \times 6$ ETF, or vertices of the icosahedron | Octahedral vertices               |
| $\mathbb{S}^{d-1}$, $N = d + 1$       | Vertices of the simplex        |                                  |
| $\mathbb{S}^{d-1}$, $N$               | $d \times N$ ETF when exists   | Open                             |

Table 2 Optimal configurations for projective Riesz kernel and best line packing when $N = 5$, $d = 3$

| $s$ | 2   | 10  | 15  | $\infty$ |
|-----|-----|-----|-----|---------|
| $\{\langle x_i, x_j \rangle : i \neq j \}$ | $[0.293, 0.506]$ | $[0.366, 0.478]$ | $[0.389, 0.471]$ | $[1/\sqrt{5} \approx 0.447]$ |

We conjecture that if $X^* = \{x_1, x_2, x_3, x_4, x_5\}$ is an optimal configuration of (1.10) for $s \in [0, \infty)$ and $N = 5$, then the cardinality of the set $\{\langle x_i, x_j \rangle, i \neq j \}$ is 2. We remark that constructions of biangular tight frames are studied in [14].

6 Optimal Configurations as Frames

We show in this section that frames rising from (1.10) are well-separated and nearly tight asymptotically. Since the frame vectors will always be on the sphere, it is understood that $\mathcal{E}_{G_s}(N)$ refers to $\mathcal{E}_{G_s}(\mathbb{S}^{d-1}, N)$.

The following theorem is the analog of Theorem 2.2 for the projective Riesz $s$-kernel. It can be over the real or complex field.

**Theorem 6.1** The best line-packing problem is the limit of problem (1.10) as $s \to \infty$:

$$
\lim_{s \to \infty} \mathcal{E}_{G_s}(N)^{1/s} = \sqrt{\frac{1}{1 - \xi_N}}.
$$

If, for $s > 0$, $X_s$ is an optimal configuration achieving $\mathcal{E}_{G_s}(N)$, then every cluster point as $s \to \infty$ of the set $\{X_s\}_{s \geq 0}$ is a Grassmannian frame.
Proof By (3.5) 

$$E_{G_s}(N) = 2^{s/2} E_{R_s}(D, N)$$

Taking the $s$th root and letting $s \to \infty$, we have

$$\lim_{s \to \infty} E_{G_s}(N)^{1/s} = \lim_{s \to \infty} \sqrt{2} E_{R_s}(D, N)^{1/s} = \frac{\sqrt{2}}{\delta_N(D)} = \sqrt{\frac{1}{1 - \xi_N}}.$$  

The last two equalities are from Theorem 2.2 and (3.9).

The second assertion is also a consequence of Theorem 2.2 since for any $G_s$-optimal configuration $\{x_i\} \subset S^{d-1}$, the configuration $\{p_i = x_i x_i^*\}$ is $R_s$-optimal for $D$. □

The Grassmannian frames have the best separation by definition, but Theorem 6.1 suggests that we are also able to find well-separated frames by solving (1.10) for large values of $s$. We will further show that projective Riesz energy minimizing frames are well-separated in the sense that their coherence have optimal order asymptotic growth (Theorem 6.3).

Let $B(x, r) \subset \mathbb{R}^m$ be the ball centered at $x$ with radius $r$. For a number $\alpha > 0$ and a positive Borel measure $\mu$ supported on $A \subset \mathbb{R}^m$, we say that $\mu$ is upper $\alpha$-regular if there is some finite constant $C_A$ such that

$$\mu(B(x, r)) \leq C_A r^\alpha$$

for all $x \in A$, $0 < r \leq \text{diam}(A)$, \hspace{1cm} (6.1)

and similarly that $\mu$ is lower $\alpha$-regular if there is some positive constant $c_A$ such that

$$\mu(B(x, r)) \geq c_A r^\alpha$$

for all $x \in A$, $0 < r \leq \text{diam}(A)$. \hspace{1cm} (6.2)

It is not difficult to verify that $\Phi_1(\sigma_{d-1})$, the uniform measure on $D$, is both upper and lower $(\dim D)$-regular (see the Appendix).

We recall that $\delta_N(D)$ is the maximum of the separation distance among all possible $N$ point configurations on $D$. Since $\Phi(\sigma_{d-1})$ is lower $(\dim D)$-regular, there is a constant $C < \infty$ such that $\delta_N(D) \leq C N^{-\frac{1}{\dim D}}$ for all $N$, which follows immediately by observing that the $\Phi(\sigma_{d-1})$ measure of an arbitrary packing in $D$ is no more than $\Phi(\sigma_{d-1})(D) = 1$. Expressing this bound in terms of coherence (recall (3.9)) gives

$$\xi_N \geq 1 - \frac{C^2}{2} N^{-\frac{2}{\dim D}}.$$  \hspace{1cm} (6.3)

The above bounds are attained by any sequence of best-packing configurations on $D$ (e.g., see [8, Chap. 13]).

Based on the above observation, we say that a sequence $(X_N)$ of $N$-point configurations in $D$ is well-separated if there is some constant $\tilde{C} > 0$ such that $\delta(X_N) \geq \tilde{C} N^{-\frac{1}{\dim D}}$ for all $N$. Equivalently, in terms of coherence, $(X_N)$ is well-separated if

$$\xi(X_N) \leq 1 - \frac{\tilde{C}}{2} N^{-\frac{2}{\dim D}},$$  \hspace{1cm} (6.4)
for all $N$.

We will show that the projective $s$-Riesz energy minimizing points are well-separated when $s > \dim \mathcal{D}$. This is a consequence of the following known theorem for optimal configurations on more general sets.

**Theorem 6.2** ([30, Corollary 2]) Suppose $A \subset \mathbb{R}^m$ is compact and supports an upper $\alpha$-regular measure $\mu$ as in (6.1). Let $s > \alpha$, $N \geq 2$ be fixed. If $X_N^*$ is an $N$-point minimizing configuration on $A$ for the $s$-Riesz energy minimizing problem (1.12), then

$$\delta(X_N^*) \geq C_1 N^{-\frac{1}{s}},$$

(6.5)

where $C_1 = \left( \frac{\mu(A)}{\alpha} \left( 1 - \frac{\alpha}{s} \right) \right)^{\frac{1}{\alpha}} \left( \frac{\alpha}{s} \right)^{\frac{1}{s}}$.

We will next apply Theorem 6.2 to obtain the following bound on the coherence of optimal $G_s$ configurations.

**Theorem 6.3** (Separation) Let $s > \dim \mathcal{D}$. If $X_s$ is an $N$-point minimizing configuration of (1.10), then

$$\xi(X_s) \leq 1 - \frac{C_2}{2} N^{-2/\dim \mathcal{D}},$$

(6.6)

where the constant $C_2$ is independent of $N$ and, in the case $\mathbb{H} = \mathbb{R}$, can be found in (6.8). Consequently, any sequence of such configurations is well-separated as $N \to \infty$.

**Proof** By (3.5), if $X_s = \{x_i\}_{i=1}^N$ is an optimal configuration of (1.10), then $P_s = \{x_i x_i^T\}_{i=1}^N$ is an optimal configuration of (3.7). Appealing to Theorem 6.2 with $A = \mathcal{D}$, the projective space embedded in $\mathbb{H} \mathbb{M}_{d \times d}^h$, and recalling that $\Phi(\sigma_{d-1})$ is upper $(\dim \mathcal{D})$-regular with constant $C_D > 0$, we have

$$\delta(P_s) \geq C_2 N^{-\frac{1}{\dim \mathcal{D}}},$$

(6.7)

where $C_2 := \left( \frac{1}{C_D (1 - \frac{\dim \mathcal{D}}{s})} \right)^{\frac{1}{\dim \mathcal{D}}} \left( \frac{\dim \mathcal{D}}{s} \right)^{\frac{1}{3}}$. The inequality (6.6) then follows from (3.8).

In the case $\mathbb{H} = \mathbb{R}$, as shown in the Appendix (see (A.4)),

$$C_D = \frac{2}{d - 1} \gamma_d = \frac{2 \Gamma(d/2)}{(d-1) \Gamma(d/2) \Gamma(1/2)},$$

where $\Gamma(\cdot)$ is the Gamma function. Therefore

$$C_2 = \frac{(d-1)(s-d+1) \Gamma(d/2) \Gamma(1/2)}{2s \Gamma(d/2)} \left( \frac{d-1}{s} \right)^{\frac{1}{3}}.$$

(6.8)

\[\Box\]
It is worth noting in the case $\mathbb{H} = \mathbb{R}$ that the expected coherence of an i.i.d. random frame $X \in S(d, N)$ generated from the uniform distribution on the sphere satisfies $\mathbb{E}[\xi(X)] \approx 1 - C_d N^{-\frac{1}{d-1}}$ (see Appendix), which is significantly worse than optimal. This fact is also demonstrated numerically in Sect. 7 (see Fig. 2).

We next show that the optimal configurations of (1.10) are nearly tight.

**Theorem 6.4** (Nearly tight) Let $s \geq 0$. If $X_N = \{x_1, \ldots, x_N\} \in S(d, N)$ is any optimal configuration for (1.10) for $N \geq 2$, then (treated as a matrix)

$$\lim_{N \to \infty} \frac{1}{N} X_N X_N^* = \frac{1}{d} I_d.$$ 

(6.9)

**Proof** Theorem 4.1(3) states that $v(\Phi(X_N)) = \frac{1}{N} \sum_{i=1}^N \delta_{\Phi(x_i)}$ converges weak* to $\Phi(\sigma_{d-1})$. Thus for every continuous function $f$ defined on $\mathcal{D}$,

$$\lim_{N \to \infty} \int_{\mathcal{D}} f d\nu(\Phi(X_N)) = \int_{\mathcal{D}} f d\Phi(\sigma_{d-1}).$$

By the definition of a pushforward measure, this can be simplified to

$$\lim_{N \to \infty} \int_{\mathbb{S}^{d-1}} f \circ \Phi d\nu(X_N) = \int_{\mathbb{S}^{d-1}} f \circ \Phi d\sigma_{d-1};$$

that is,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N f(\Phi(x_i)) = \int_{\mathbb{S}^{d-1}} f(\Phi(x)) d\sigma_{d-1}. \quad (6.10)$$

Let $f(\Phi(x)) = xx^*$ be a vector-valued function. Then (6.10) implies

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N x_i x_i^* = \int_{\mathbb{S}^{d-1}} xx^* d\sigma_{d-1}. \quad (6.11)$$

We need to integrate every entry of the right-hand side. Let $x = (x(1), x(2), \ldots, x(d))^T \in \mathbb{S}^{d-1}$, so that $xx^* = (x(i)x(j))$. Then,

- if $i = j$, $\int |x(j)|^2 d\sigma_{d-1} = \frac{1}{d} \int (|x(1)|^2 + \cdots + |x(d)|^2) d\sigma_{d-1} = \frac{1}{d}$;
- if $i \neq j$, $\int x(i)x(j) d\sigma_{d-1} = 0$ by symmetry.

Since $X_N X_N^* = \frac{1}{N} \sum_{i=1}^N x_i x_i^*$, from (6.11) we deduce that

$$\lim_{N \to \infty} \frac{1}{N} X_N X_N^* = \frac{1}{d} I_d.$$

$\square$
Theorem 6.4 says that the optimal configurations are nearly tight asymptotically as $N \to \infty$ in relation to (1.1). More desirable would be a stronger result of the form

$$\|X_N X_N^* - \frac{N}{d} I_d\|_F = O(N^{-q}), \quad q > 0. \quad (6.12)$$

The numerical experiments in Sect. 7 (left side of Fig. 3) do indeed suggest a result like (6.12) holds at least for small values of $s$. The work [9] provides a partial explanation for this phenomenon. It studies the convergence rate of (6.10) for $f$ in a Sobolev space (which is the case for every entry of $xx^*$). The numerical experiments therein suggests that the $s$-Riesz minimizing configurations (when $s = 0, 1$) achieve the optimal order quasi Monte Carlo error bounds.

Regarding random tight frames, it is shown in [22, Corollary 3.21] that

$$\mathbb{E}\left(\|X_N X_N^* - \frac{N}{d} I_d\|_F^2\right) = N\left(1 - \frac{1}{d}\right),$$

which grows as $N$ grows. Section 7 (right of Fig. 3) shows that optimal configurations of (1.10) also outperforms random configurations on tightness.

### 7 Numerical Experiments

The numerical experiments conducted consider points in the real vector space, and were executed in Matlab. When solving (1.10) (or (1.13) for negative $s$), spherical coordinates are used so that the command `fminunc` (unconstrained minimization) can be employed. Four experiments were performed.

The first and the second experiments deal with the separation and tightness of the optimal configurations of (1.10) or (1.13), and are explained in Sects. 7.1 and 7.2. Since the objective function has lots of local minima, in both experiments, we run `fminunc` with multiple random initializations to obtain a putative minimum. We then test whether the optimal configurations are nearly tight or have small coherence (well-separatedness).

The third experiment presents an algorithm for obtaining tight frames with good separation. As explained in Sect. 7.3, it is crucial to use a well-separated frame as an initialization.

#### 7.1 Good Separation

The first experiment explores the asymptotic behavior of the coherence $\xi(X) = \max_{i \neq j} |\langle x_i, x_j \rangle|$ of projective Riesz minimizing points for various values of $s$ as $N$ gets larger. The result displayed in Fig. 1 is for $d = 3$ with points on $S^2$. The number of points $N$ ranges from 3 to 100. The separation result Theorem 6.3 only applies to $s > 2$, but our numerical experiment shows that the log case and $s = 1$ case are achieving smaller coherence. The $s = -2$ (frame potential) case has the worst behavior as its minimizers could contain repeated (or antipodal) points. Notice that the
coherence gets smaller as $s$ increases which is consistent with Theorem 6.1. Finally, the coherence curve was fit with $y = 1 - 3/N$, which reflects Theorem 6.3.

The second experiment computed the coherence of the projective Riesz minimizing points for $d = 6$ and relatively small values of $N$ (from 6 to 40), as shown in Fig. 2. Various $s$ are computed and compared with the Welch bound (5.1), the Levenstein bound [36,42]

$$
\xi(X) \geq \sqrt{\frac{3N - d^2 - 2d}{(d + 2)(N - d)}} \quad \text{if } N > d(d + 1)/2,
$$

and the Sloane database http://neilsloane.com/grass/. The Sloane database has the best known line-packings or the smallest coherence given $d, N$, among which some are only putatively known. Figure 2 also includes uniform random configurations. For each $N$, we display the coherence that is averaged over 20 samples. We again observe that larger $s$ produces better separated frames, and $s = -2$ (frame potential case) produces highly correlated frames. For all values of $s$ except for $-2$, (1.10) achieves the Welch bound when $N = 6, 7, 16$ (these are all the ETFs and thus universally optimal), and it achieves the Levenstein bound when $N = 36$. The 36 point configuration in $\mathbb{R}^6$ is the 6-dimensional lattice $E_6$ [26] and is also known to be universally optimal [19] although not an ETF. We further remark that our numerical experiments suggest that the Sloane grassmannian configurations for $d = 6$ and $N = 12$ and $N = 22$ may be universally optimal. This might also be anticipated from Figs 2 and 4. These figures might also suggest the universal optimality of the Sloane configuration for $N = 21$, however this turns out not to be the case.

7.2 Nearly Tight

We addressed the tightness of the optimal configurations by computing $\|XX^T - \frac{N}{d} I_d\|_F$. We reuse the points generated from the first experiment with $d = 3$ and $N$
Fig. 2 Coherence of projective riesz optimal configuration for $d = 6$ with various values of $s$

Fig. 3 Tightness for $d = 3$. The right side plot includes random configurations ranging from 3 to 100. Figure 3 (left) shows the results for $s = -2, -1, 0, 1, 2, 3$. The $s = -2$ (frame potential) case recovers tight frames since by (5.2), Riesz $(-2)$-energy is equal to $\|XX^T - \frac{N}{d}I_d\|_F^2$ plus a constant. Unfortunately, the separation property deteriorates as $s$ decreases while the tightness property improves. This is further validated by the poor tightness of the Sloane points as they correspond to the $s = \infty$ case. A least squares curve fitting was also performed for the peaks (least tight) for $s = 1$, which exhibits an $N^{-1/2}$ decay, a better rate than what Theorem 6.4 guarantees. Notice that the right side of Fig. 3 also includes uniform random vectors
for comparison. The randomly generated configurations exhibit worse behavior for both coherence and tightness. This has also been observed in [9].

The tightness for \( d = 6 \) with \( N \) ranging from 6 to 40 is illustrated in Fig. 4 where the points generated from the second experiment are reused. The figure displays a clear pattern of improved tightness as \( s \) decreases.

### 7.3 Achieving Good Separation and Exact Tightness

In this section we present experiments based on a simple algorithm for obtaining frames with good separation and exact tightness. For the frame potential minimization problem (\( s = -2 \) of (1.13)), recall that every local minimizer is a global minimizer; i.e., a tight frame [2]. The output of \texttt{fminunc}” is certainly affected by the initial input. As seen in Figs. 1 and 2, the tight frames found by minimizing the frame potential using random initializations generically have poor separation. We propose the following approach for generating well-separated tight frames in \( S(d, N) \) for given \( d \) and \( N \).

1. Generate a random frame \( X \in S(d, N) \).
2. Using \( X \) as an initial configuration, use an optimization algorithm (such as gradient descent) to find a local minimizer \( Y \) for (1.10) for some \( s > d - 1 \). Motivated by Theorems 6.3 and 6.4 the minimizer \( Y \) is expected to be well-separated and nearly tight.
3. Minimize (1.13) with \( s = -2 \) using \( Y \) as the initial configuration. The experiments presented below suggest that the resulting frame is well-separated and tight.

Variations on this approach such as iterating steps 2 and 3 or minimizing Riesz-\( s \) energy restricted to the manifold of tight frames will be explored in future work.

Figure 5 shows the performance of the optimal configuration of minimizing frame potential with the initialization being the optimal configuration obtained through solving (1.10). The numerics indicate that these optimal tight configurations are indeed
well-separated. The left graph of Fig. 5 should be compared to Fig. 2 (the values of $s$ used in step 2 of the above algorithm are indicated in the figure and include values of $s < d - 1$). Numerically, this is a promising way to find well-separated tight frames, which has many applications including signal transmission [27,32].

The set of finite unit norm frames is topologically connected, and an irreducible variety [11], but our experiment suggests that for a local minima of (1.10), there will be a tight frame close to it. This can perhaps be explained by the recently solved Paulsen Problem [29], which implies that for a nearly tight unit norm frame $F$, there exists a unit norm tight frame nearby since we have shown that a local minima of (1.10) is nearly tight. This suggests that step 3 will result in a nearby tight configuration if the configuration from step 2 is nearly tight as indicated in Theorem 6.4 for $N$ large.

To further see how the initializations impact the frame potential problem, Fig. 6 compares the coherence of the optimal configuration of solving (1.13) ($s = -2$)
Fig. 7  $F^{-1}(B(p_x, r))$

with different initializations. The results are similar, but note that starting with Sloane points, the best separated points among the three, does not necessarily end up with the best separation.

Appendix A

Uniform Measure

Given the hypersphere $S^{d-1}$, let $C_r(x)$ be the hyperspherical cap centered at $x$, with $r$ being the Euclidean distance of the furthest point to $x$. That is,

$$C_r(x) = \{y \in S^{d-1} : \|x - y\| \leq r\}.$$

Recalling that $\sigma_{d-1}$ denotes the normalized surface measure, the following asymptotic formula holds:

$$\sigma_{d-1}(C_r(x)) = \frac{1}{d-1} \gamma_d r^{d-1} + O(r^{d+1}), \quad (r \to 0),$$

(A.1)

and also the estimate

$$\sigma_{d-1}(C_r(x)) \leq \frac{1}{d-1} \gamma_d r^{d-1},$$

(A.2)

where

$$\gamma_d := \frac{\Gamma(d/2)}{\Gamma((d-1)/2)\Gamma(1/2)}.$$

(A.3)

Both estimates can be found in Sect. 3 of [33].

Lemma A.1 When $\mathbb{H} = \mathbb{R}$, the uniform measure on $\mathcal{D}$ is $(d-1)$-regular. Moreover, we have the estimate

$$\Phi(\sigma_{d-1})(B(p_x, r)) \leq \frac{2}{d-1} \gamma_d r^{d-1}, \quad \text{for any } p_x \in \mathcal{D}, 0 < r \leq \text{diam}(\mathcal{D})$$

(A.4)

Proof $\mathcal{D}$ is the projective space embeded in $\mathbb{R}M^h_{d \times d}$. $p_x$ and $p_y$ are furthest away if $x \perp y$, so $\text{diam}(\mathcal{D}) = \sqrt{2}$.

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For any point $p_x = F(x) \in D$ and any $r \leq \text{diam}(D) = \sqrt{2}$, suppose in the set $B(p_x, r) \cap D$, $p_y$ is the point that is furthest away from $p_x$. We can pick $y$ so that $\langle x, y \rangle \geq 0$. Then $\Phi^{-1}(B(p_x, r))$ is the union of the spherical cap centered at $x$ with boundary point $y$ together with its antipodal image, see Fig. 7. By (3.3),

$$
|\langle x, y \rangle|^2 = 1 - \|p_x - p_y\|^2 / 2 \geq 1 - r^2 / 2,
$$

$$
||x - y||^2 = 2 - 2\langle x, y \rangle \leq 2 - 2\sqrt{1 - r^2 / 2} \leq 2 - 2(1 - r^2 / 2) = r^2.
$$

By (A.2),

$$
\Phi(\sigma_{d-1})(B(p_x, r)) = \sigma_{d-1}(\Phi^{-1}(B(x, r))) = 2\sigma_{d-1}(C_r(x)) \leq \frac{2}{d-1} \kappa_d r^{d-1}.
$$

\[\square\]

### A.1 Expected Value of Coherence

Let $X = \{x_i\} \in S(d, N)$ be a random configuration on the sphere where each point is selected from a uniform distribution on the sphere. Let $\Theta = \min_{i \neq j} \arccos \langle x_i, x_j \rangle$, so

$$
\xi(X) = \max_{i \neq j} |\langle x_i, x_j \rangle| \geq \max_{i \neq j} \langle x_i, x_j \rangle = \cos \Theta \geq 1 - \Theta^2 / 2. \quad (A.5)
$$

It is proven in [12, Theorem 2] that $F_N(t) := \Pr(N^{2/(d-1)} \Theta \leq t) \to F(t)$ where $F(t) = 1 - \exp\left(-\frac{\kappa_d}{2(d-1)} t^{d-1}\right)$ is supported on $(0, \infty)$.

In order to compute the expected value of $\Theta^2$, we define $G_N(s) := \Pr(N^{4/(d-1)} \Theta^2 \leq s) = F_N(\sqrt{s}) \to F(\sqrt{s})$. By a similar argument as the one in [10, Corollary 3.4], we get

$$
\lim_{N \to \infty} \mathbb{E}(N^{4/(d-1)} \Theta^2) = \lim_{N \to \infty} \int_0^\infty (1 - G_N(s)) ds = \int_0^\infty 1 - F(\sqrt{s}) ds = \int_0^\infty \exp\left(-\frac{1}{2} \kappa_d s^{d-1}\right) = C_d.
$$

By (A.5), we have

$$
\mathbb{E}(\xi(X)) \geq \mathbb{E}(1 - \Theta^2 / 2) \sim 1 - \frac{C_d}{2} N^{-4/(d-1)}.
$$

### References

1. Bachoc, F., Ehler, M., Gräf, M.: Optimal configurations of lines and a statistical application. Adv. Comput. Math. 43(1), 113–126 (2017)
2. Benedetto, J., Fickus, M.: Finite normalized tight frames. Adv. Comput. Math. 18(2–4), 357–385 (2003)
3. Benedetto, J., Kolesar, J.D.: Geometric properties of Grassmannian frames for $\mathbb{R}^2$ and $\mathbb{R}^3$. EURASIP J Adv. Signal Process 1, 049850 (2006)
4. Bétermin, L., Sandler, E.: Renormalized energy and asymptotic expansion of optimal logarithmic energy on the sphere. Constr. Approx. 47(1), 39–74 (2018)
5. Bilyk, D., Glazyrin, A., Matzke, R., Park, J., Vlasiuk, O.: Optimal measures for $p$-frame energies on spheres. arXiv preprint arXiv:1908.00885 (2019)
6. Bodmann, B.G., Haas, J.I.: Frame potentials and the geometry of frames. J. Fourier Anal. Appl. 21, 1344–1384 (2014)
7. Borodachov, S.V., Hardin, D.P., Saff, E.B.: Asymptotics for discrete weighted minimal Riesz energy problems on rectifiable sets. Trans. Am. Math. Soc. 360(3), 1559–1580 (2008)
8. Borodachov, S.V., Hardin, D.P., Saff, E.B.: Discrete Energy on Rectifiable Sets. Springer, New York (2019)
9. Brauchart, J.S., Saff, E.B., Sloan, I.H., Womersley, R.S.: QMC designs: optimal order Quasi Monte Carlo integration schemes on the sphere. Math. Comput. 83(290), 2821–2851 (2014)
10. Brauchart, J.S., Reznikov, A.B., Saff, E.B., Sloan, I.H., Wang, Y.G., Womersley, R.S.: Random point sets on the sphere-hole radii, covering, and separation. Exp. Math. 27(1), 62–81 (2018)
11. Cahill, J., Mixon, D.G., Strawn, N.: Connectivity and irreducibility of algebraic varieties of finite unit norm tight frames. SIAM J. Appl. Algebra Geom. 1(1), 38–72 (2017)
12. Cai, T., Fan, J., Jiang, T.: Distributions of angles in random packing on spheres. J. Mach. Learn. Res. 14(1), 1837–1864 (2013)
13. Candes, E., Strohmer, T., Voroninski, V.: Phaselift: exact and stable signal recovery from magnitude measurements via convex programming. Commun. Pure Appl. Math. 66(8), 1241–1274 (2013)
14. Casazza, P.G., Cahill, J., Haas, J.I., Treiman, J.: Constructions of biangular tight frames and their relationships with equiangular tight frames. arXiv preprint arXiv:1703.01786 (2017)
15. Chen, X., Powell, A.M.: Random subspace actions and fusion frames. Constr. Approx. 43(1), 103–134 (2016)
16. Chen, X., Gonzalez, V., Goodman, E., Kang, S., Okoudjou, K.: Universal optimal configurations for the $p$-potential frames. Adv. Comput. Math. 46, 4 (2020)
17. Choquet, G.: Diametre transfini et comparaison de diverses capacités. Sémin. Brelot Choquet Deny. Théorie Potentiel 3(4), 1–7 (1958)
18. Cohn, H., Kumar, A.: Universally optimal distribution of points on spheres. J. Am. Math. Soc. 20(1), 99–148 (2007)
19. Cohn, H., Kumar, A., Minton, G.: Optimal simplices and codes in projective spaces. Geom. Topol. 20(3), 1289–1357 (2016)
20. Conway, J.H., Hardin, R.H., Sloane, N.J.A.: Packing lines, planes, etc.: packings in Grassmannian spaces. Exp. Math. 5(2), 139–159 (1996)
21. Delsarte, P., Goethals, J.M., Seidel, J.J.: Bounds for systems of lines, and Jacobi polynomials. Geom. Comb. 30, 193–207 (1991)
22. Ehler, M.: Random tight frames. J. Fourier Anal. Appl. 18(1), 1–20 (2012)
23. Ehler, M., Okoudjou, K.: Minimization of the probabilistic $p$-frame potential. J. Stat. Plan. Inference 142(3), 645–659 (2012)
24. Fejes, L., Tóth, L.: On the sum of distances determined by a pointset. Acta Math. Hungar. 7(3–4), 397–401 (1956)
25. Fickus, M., Mixon, D.G.: Tables of the existence of equiangular tight frames. arXiv preprint arXiv:1504.00253 (2015)
26. Fickus, M., Jasper, J., Mixon, D.G.: Packings in real projective spaces. SIAM J Appl. Algebra Geom. 2(3), 377–409 (2018)
27. Goyal, V.K., Kovačević, J., Kelner, J.A.: Quantized frame expansions with erasures. Appl. Comput. Harmon. Anal. 10(3), 203–233 (2001)
28. Gross, D., Krahmer, F., Kueng, R.: A partial derandomization of phaselift using spherical designs. J. Fourier Anal. Appl. 21(2), 229–266 (2015)
29. Hamilton, L., Moitra, A.: The Paulsen problem made simple. In: Proceedings of the 10th Annual Innovations in Theoretical Computer Science (ITCS 2019)
30. Hardin, D.P., Saff, E.B., Whitehouse, J.T.: Quasi-uniformity of minimal weighted energy points on compact metric spaces. J. Complex. 28(2), 177–191 (2012)
31. Hardin, D.P., Leblé, T., Saff, E.B., Serfaty, S.: Large deviation principles for hypersingular Riesz gases. Constr. Approx. 48(1), 61–100 (2018)
32. Holmes, R.B., Paulsen, V.I.: Optimal frames for erasures. Linear Algebra Appl. 377, 31–51 (2004)
33. Kuijlaars, A.B.J., Saff, E.B.: Asymptotics for minimal discrete energy on the sphere. Trans. Am. Math. Soc. 350(2), 523–538 (1998)
34. Landkof, N.S.: Foundations of Modern Potential Theory. Springer, New York (1972)
35. Lee, J.M.: Introduction to Smooth Manifolds, pp. 1–29. Springer, New York (2003)
36. Levenshtein, V.I.: Designs as maximum codes in polynomial metric spaces. Acta Appl. Math. 29(1–2), 1–82 (1992)
37. Mattila, P.: Geometry of Sets and Measures in Euclidean Spaces: Fractals and Rectifiability, vol. 44. Cambridge University Press, Cambridge (1999)
38. Schwartz, R.E.: Five point energy minimization: a synopsis. Constr. Approx. 51, 537–564 (2020)
39. Strohmer, T., Heath Jr., R.W.: Grassmannian frames with applications to coding and communication. Appl. Comput. Harmon. Anal. 14(3), 257–275 (2003)
40. Sustik, M.A., Tropp, J.A., Dhillon, I.S., Heath Jr., R.W.: On the existence of equiangular tight frames. Linear Algebra Appl. 426(2–3), 619–635 (2007)
41. Welch, L.: Lower bounds on the maximum cross correlation of signals (Corresp). IEEE Trans. Inform. Theory 20(3), 397–399 (1974)
42. Zhou, Z., Ding, C., Li, N.: New families of codebooks achieving the Levenstein bound. IEEE Trans. Inform. Theory 60(11), 7382–7387 (2014)

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