UNIVERSAL OPTIMAL CONFIGURATIONS FOR THE p-FRAME POTENTIALS

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ABSTRACT. Given $d, N \geq 2$ and $p \in (0, \infty]$ we consider a family of functionals, the p-frame potentials $\mathrm{FP}_{p,N,d}$, defined on the set of all collections of N unit-norm vectors in $\mathbb{R}^d$. For the special cases $p = 2$ and $p = \infty$, both the minima and the minimizers of these potentials have been thoroughly investigated. In this paper, we investigate the minimizers of the functionals $\mathrm{FP}_{p,N,d}$, by first establishing some general properties of their minima. Thereafter, we focus on the special case $d = 2$, for which, surprisingly, not much is known. One of our main results establishes the unique minimizer for big enough p. Moreover, this minimizer is universal in the sense that it minimizes a large range of energy functions that includes the p-frame potential. We conclude the paper by reporting some numerical experiments for the case $d \geq 3$, $N = d + 1$, $p \in (0, 2)$. These experiments lead to some conjectures that we pose.

Keywords: Potential energy minimization, Frame potential, Sharp configuration, Spherical designs

1. INTRODUCTION

A set of vectors $X = \{x_k\}_{k=1}^N \subseteq \mathbb{R}^d$ is a *frame* for $\mathbb{R}^d$ if there exist $0 < A \leq B < \infty$ such that

$$A\|x\|^2 \leq \sum_{k=1}^{N} |\langle x, x_k\rangle|^2 \leq B\|x\|^2 \quad \text{for all } x \in \mathbb{R}^d, \tag{1}$$

where $\|\cdot\|$ denotes the Euclidean norm. If, in addition, each x_k is unit-norm, we say that X is a *unit-norm frame*. X is called *tight* if $A = B$. A tight unit-norm frame is called a *finite unit-norm tight frame (FUNTF)*. One attractive feature of FUNTFs is the fact that they can be used to decompose and reconstruct any vector x via the following formula:

$$x = \frac{d}{N} \sum_{k=1}^{N} \langle x, x_k\rangle x_k. \tag{2}$$

Frames in general, and FUNTFs in particular, are routinely used in many applications, especially in signal processing. For more on the theory and the applications of frames we refer to [10, 18, 19, 20].

A frame X is said to be *equiangular* if there exists $c > 0$ such that

$$\left|\left\langle \frac{x_k}{\|x_k\|}, \frac{x_l}{\|x_l\|} \right\rangle\right| = c \quad \text{for all } k \neq l.$$

If in addition X is tight, then X is called an *equiangular tight frame (ETF)*. It follows from [8, Proposition 1.2] that the vectors of an ETF have necessarily equal norm. Consequently,

2010 *Mathematics Subject Classification.* Primary 42C15 52C17 74G65; Secondary 41A05 52A40 .

and without loss of generality, all ETFs considered in the sequel will be unit-norm frames, i.e., FUNTFs.

Let $S(N,d)$ be the collection of all sets of N unit-norm vectors. For any $p \in (0,\infty]$, the *p-frame potential* of $X = \{x_k\}_{k=1}^N \in S(N,d)$ is defined as

$$\mathrm{FP}_{p,N,d}(X) := \begin{cases} \displaystyle\sum_{k=1}^{N}\sum_{\ell\neq k}^{N} |\langle x_k, x_\ell\rangle|^p, & \text{when } p<\infty \\ \displaystyle\max_{k\neq\ell} |\langle x_k, x_\ell\rangle|, & \text{when } p=\infty. \end{cases} \tag{3}$$

The definition of the p-frame potential above differs from the one given in [15] as (3) excludes self inner products. As will be seen in Section 2, the present definition will allow us to state our results in a more concise manner. The subscripts N, d are a little redundant since they are suggested by the input X, but they will come in handy when we want to emphasize the dimension or the number of points. We are interested in finding the infimum of the p-frame potential among all N-point configurations in $S(N,d)$. It is a standard argument to show that this infimum can be achieved due to the compactness of the sphere and the continuity of the function, so we can replace infimum by minimum and define

$$\mathcal{F}_{p,N,d} := \min_{X\in S(N,d)} \mathrm{FP}_{p,N,d}(X). \tag{4}$$

In situations when N, d are both fixed, we will simply use $\mathcal{F}_p$ for $\mathcal{F}_{p,N,d}$, and FP_p for $\mathrm{FP}_{p,N,d}$. Similarly we use the notations $\mathcal{F}_N, \mathrm{FP}_N$ if p and d are fixed. Any minimizer of (4) will be called an *optimal configuration* of the p-frame potential. We observe that if $X^* = \{x_1^*, \cdots, x_N^*\}$ is optimal, then with any orthogonal matrix U, any permutation π, and any $s_i \in \{1,-1\}$,

$$\{s_1 U x_{\pi_1}^*, \cdots, s_N U x_{\pi_N}^*\}$$

is optimal too. In other words, the optimal configuration is an equivalence class with respect to orthogonal transformations, permutations or sign switches. So when we say an optimal configuration is unique, we mean that it is unique up to this equivalence relation.

Note that in the definition of the frame potential, X does not necessarily need to be a frame of $\mathbb{R}^d$, but we will show in Proposition 2.1 that the minimizers of the p-frame potential must be a frame, as expected. Therefore problem (4) remains the same if we had restricted X to be a unit-norm frame with N frame vectors.

The name "frame potential" originates from the special case $p = 2$,

$$\mathrm{FP}_{2,N,d}(X) = \sum_{k=1}^{N}\sum_{l\neq k}^{N} |\langle x_k, x_l\rangle|^2 \tag{5}$$

which was studied by Benedetto and Fickus [3]. They proved that X^* is an optimal configuration of $\mathrm{FP}_{2,N,d}(X)$ if and only if $X^* = \{x_k^*\}_{k=1}^N$ is a FUNTF.

Another important special case is $p = \infty$. In this case, the quantity

$$c(X) := \mathrm{FP}_{\infty,N,d}(X) = \max_{k\neq\ell} |\langle x_k, x_\ell\rangle| \tag{6}$$

is also called the *coherence* of $X = \{x_k\}_{k=1}^N \in S(N,d)$, and its minimizers are called *Grassmannian frames* [4, 5, 9, 23, 26]. The following Welch bound [26] is well known:

$$\mathrm{FP}_{\infty,N,d}(X) \geq \sqrt{\frac{N-d}{d(N-1)}}, \tag{7}$$

and the equality in (7) holds if and only if $X = \{x_k\}_{k=1}^N$ is an ETF, which is only possible if $N \leq \dfrac{d(d+1)}{2}$ [13]. The coherence minimization problem corresponds to $p = \infty$ because it appears to be the limiting case when p grows to infinity; see Proposition 2.2. It is known that ETFs, when they exist, are minimizers of (3) for $p > 2$ [15, 7].

When p is an even integer, the minimizers of $\mathrm{FP}_{p,N,d}$ have long been investigated in the setting of spherical designs, see [22, 15, 25]. A set of N points $X \subset \mathbb{S}^{d-1}$ (the unit sphere in $\mathbb{R}^d$) is called a spherical t-design if for every homogeneous polynomial h of degree t or less,

$$\int_{\mathbb{S}^{d-1}} h(\xi) d\sigma(\xi) = \frac{1}{N} \sum_{x \in X} h(x),$$

where σ is the normalized surface measure on $\mathbb{S}^{d-1}$. For example, a spherical 1-design is a set of points whose center of mass is at the origin. More generally, as shown in [15] or [25, Theorem 8.1], if p is an even integer and $X \in S(N,d)$ is symmetric, that is $X = -X$, then

$$\mathrm{FP}_{p,N,d}(X) \geq N^2 \frac{1 \cdot 3 \cdot 5 \cdots (p-1)}{d(d+2)\cdots(d+p-2)} - N, \tag{8}$$

and equality holds if and only if X is a spherical p-design.

Optimal configurations of (4) are often not symmetric since x_i and $-x_i$ are considered the same points as far as frame potential is concerned. However, we can still use (8) by symmetrizing a frame. Given $X = \{x_i\}_{i=1}^N$ such that its coherence $c(X) < 1$ (i.e. no repeated vectors or opposite vectors), we let

$$X^{sym} := \{x_i\}_{i=1}^N \cup \{-x_i\}_{i=1}^N \in S(2N,d).$$

Some straightforward computations result in

$$\mathrm{FP}_{p,2N}(X^{sym}) = 4\mathrm{FP}_{p,N}(X) + 2N \tag{9}$$

which combined with (8), can be used to prove

Proposition 1.1. *Let p be an even integer, then*

$$FP_{p,N,d}(X) = \frac{1}{4}(FP_{p,2N}(X^{sym}) - 2N) \geq N^2 \frac{1 \cdot 3 \cdot 5 \cdots (p-1)}{d(d+2)\cdots(d+p-2)} - N,$$

and equality holds if and only if X^{sym} is a spherical p-design.

Not only is Proposition 1.1 limited to even p's, but it is also not trivial to find spherical t-designs for large t. More generally, and to the best of our knowledge, little is known about the complete solutions to (4) even in the simplest case $d = 2$. When $N = 3$, a solution is given in [15] for all positive p. See also [6, 21] for related results. For any N and $p = \infty$, it is shown in [5] that the Grassmannian frame is

$$X_N^{(h)} = \left\{ \begin{bmatrix} \cos 0 \\ \sin 0 \end{bmatrix}, \begin{bmatrix} \cos \frac{\pi}{N} \\ \sin \frac{\pi}{N} \end{bmatrix}, \begin{bmatrix} \cos \frac{2\pi}{N} \\ \sin \frac{2\pi}{N} \end{bmatrix}, \cdots, \begin{bmatrix} \cos \frac{(N-1)\pi}{N} \\ \sin \frac{(N-1)\pi}{N} \end{bmatrix} \right\}, \tag{10}$$

which can be viewed as N equally spaced points on the half circle. The main result of this paper establishes that the unique optimal configuration when $d = 2$, $N \geq 4$, and $p > 4\lfloor \frac{N}{2} \rfloor - 2$ is $X_N^{(h)}$, where $\lfloor c \rfloor$ is the largest integer that does not exceed c. Moreover for $N = 4$, our result is sharper as we prove this is the case for $p > 2$. Such a result is expected since optimal configurations for large p are approaching the Grassmannian frame. Moreover, we are able to show that $X_N^{(h)}$ is the optimal configuration for a big class of kernel functions. See Theorem 3.5. The phenomenon that a given configuration is the optimal configuration for a large range of functions is what we call universal. Such a name stems from the work [12]. In addition to these results, we present numerical results for all other values of p and N when $d = 2$. Finally, we also consider the special case of $N = d + 1$ and $d \geq 3$ and state a conjecture regarding the function $\mathcal{F}_p$ for $p \in (0, 2]$. Based on the results of the present paper, Table 1 gives the state of affairs concerning the solutions of (4) and is an invitation to initiate a broader discussion on the problem. We would like to remark that the case $N = d + 1$ has been solved by others during the revision of this manuscript; see Section 4 for more details.

The rest of the paper is organized as follows. Section 2 states some basic results of the p-frame potential including some asymptotic results as $N \to \infty$. Section 3 presents the results for $d = 2$. Section 4 presents conjectures and numerical results for the case $N = d + 1$. Throughout the paper, we will use $[m : n]$ for the index set $\{m, m + 1, \cdots, n\}$.

TABLE 1. Optimal configurations for the p-frame potential

	$\mathbb{R}^2$	$\mathbb{R}^d$
$p \in (0, \frac{\ln 3}{\ln 2})$	$N = 3$: ONB+ [15]	$N = d + 1$: ONB+ [17]
$p \in (\frac{\ln 3}{\ln 2}, 2)$	$N = 3$: ETF [15]	$N = d + 1$: see Conjecture 4.5
$p \in (0, 2)$	$N = 2k$: k copies of ONB [15]	$N = kd$: k copies of ONB [15]
$p = 2$	FUNTF [3]	
$p \in (4\lfloor \frac{N}{2} \rfloor - 2, \infty)$	$N \geq 5 : X_N^{(h)}$ (Theorem 3.7)	ETF if exists [15, 23]
$p = \infty$	Any N: $X_N^{(h)}$ [5]	
$p \in (2, \infty)$	$N = 4$: $X_4^{(h)}$ (Theorem 3.7)	

ONB+ refers to an orthonormal basis with a repeated vector. See Definition 4.1(a).

2. Some basic results

Intuitively, minimizing the frame potential amounts to promoting big angles among vectors. Consequently, it is expected that the optimal configurations will be at least a frame whose vectors are reasonably spread out in the sphere. If X is not a frame, then one can always find a vector e that is orthogonal to X, and replacing any vector in X by e won't increase the frame potential. In other words, it is trivial to show that problem (4) might as well be restricted to frames. The following result shows something stronger, that is, it excludes the possibility that a minimizer doesn't span $\mathbb{R}^d$.

Proposition 2.1. *For $p \in (0, \infty]$, any optimal configuration of (4) is a frame of $\mathbb{R}^d$.*

Proof. We first consider the case $p \in (0, \infty)$. Suppose not, and say $X^* = \{x_k^*\}_{k=1}^N \subset \mathbb{S}^{d-1}$ is a minimizer so that $\operatorname{span} X^*$ is a strict subset of $\mathbb{R}^d$. Because there are $N \geq d$ vectors, it is possible to select two indices k_1 and k_2 such that $|\langle x_{k_1}^*, x_{k_2}^* \rangle| > 0$. Finally, select any unit-norm vector $x_0 \in (\operatorname{span} X^*)^\perp$ and replace $x_{k_1}^*$ with x_0; i.e., define $Y = \{x_k^*\}_{k \neq k_1} \cup \{x_0\}$. A direct computation shows that $\mathrm{FP}_{p,M,N}(Y) < \mathrm{FP}_{p,M,N}(X^*)$.

Now consider the case $p = \infty$ and let $X^* = \{x_k^*\}_{k=1}^N \subset \mathbb{S}^{d-1}$ be a minimizer of $\mathrm{FP}_{\infty,N,d}$. Suppose that the dimension of $\operatorname{span}(X^*) \leq d-1$. Choose a unit vector $e \in (\operatorname{span} X^*)^\perp$. There could be multiple pairs of vectors that achieve the maximal inner product $\mathcal{F}_\infty = \mathrm{FP}_{\infty,N,d}(X^*)$. Without loss of generality, we assume these vectors are among the first K vectors, that is,

$$|\langle x_i^*, x_j^* \rangle| < \mathcal{F}_\infty, \quad \text{if either } i \text{ or } j \text{ does not belong to } [1:K], i \neq j. \tag{11}$$

We will construct $Y = \{y_k\}_{k=1}^K \cup \{x_k^*\}_{k=K+1}^N$ that will have smaller coherence.

For $i = 1, 2, \cdots, K$, let $y_i = \sqrt{1-\epsilon_i} x_i^* + \sqrt{\epsilon_i} e$, where $0 < \epsilon_i < 1$. Define

$$f(a,b) := \frac{\sqrt{a}\sqrt{b}}{1 - \sqrt{1-a}\sqrt{1-b}} \text{ on } (0,1] \times (0,1].$$

If we choose ϵ_i, ϵ_j such that

$$f(\epsilon_i, \epsilon_j) = \frac{\sqrt{\epsilon_i}\sqrt{\epsilon_j}}{1 - \sqrt{1-\epsilon_i}\sqrt{1-\epsilon_j}} < \mathcal{F}_\infty, \tag{12}$$

then

$$|\langle y_i, y_j \rangle| = |\sqrt{1-\epsilon_i}\sqrt{1-\epsilon_j}\langle x_i^*, x_j^* \rangle + \sqrt{\epsilon_i}\sqrt{\epsilon_j}| \leq \sqrt{1-\epsilon_i}\sqrt{1-\epsilon_j}\mathcal{F}_\infty + \sqrt{\epsilon_i}\sqrt{\epsilon_j} < \mathcal{F}_\infty. \tag{13}$$

We will pick ϵ_i iteratively to satisfy (12):
Step 1: pick $0 < \epsilon_1 < 1$ arbitrarily.
Step i: given $\epsilon_1, \cdots, \epsilon_{i-1}$, pick $\epsilon_i > 0$ such that $f(\epsilon_j, \epsilon_i) < \mathcal{F}_\infty$, for all $j = 1, \cdots, i-1$. This is possible because $\lim_{\epsilon \to 0} f(\epsilon_j, \epsilon) = 0$ for all $j \leq i-1$.

For convenience, let $y_k = x_k^*$ for $k = K+1, \cdots, N$. The new frame $Y = \{y_k\}_{k=1}^K$ has a smaller coherence because for any pair i, j, if $i, j \in [1:K]$, then $|\langle y_i, y_j \rangle| < \mathcal{F}_\infty$ by (13); if $i, j \in [K+1:N]$, then $|\langle y_i, y_j \rangle| = |\langle x_i^*, x_j^* \rangle| < \mathcal{F}_\infty$ by (11); if $i \in [1:K], j \in [K+1:N]$, then $|\langle y_i, y_j \rangle| = |\langle \sqrt{1-\epsilon_i} x_i^* + \sqrt{\epsilon_i} e, x_j^* \rangle| = \sqrt{1-\epsilon_i}|\langle x_i^*, x_j^* \rangle| < \mathcal{F}_\infty$.

This is a contradiction, so the optimal configuration must be a frame. □

Now we establish the relationship between large p and $p = \infty$.

Proposition 2.2. $\lim_{p \to \infty} \mathcal{F}_p^{1/p} = \mathcal{F}_\infty$. *Moreover, if $X^{(p)}$ is an optimal configuration for* (4) *when $p < \infty$ and X is a cluster point of the set $\{X^{(p)}\}_{p>0}$, then X optimizes the coherence as $X = \arg\min_{Y \in S(N,d)} c(Y)$.*

Proof. On one hand, we have

$$\mathcal{F}_p^{1/p} = \left(\sum_{i \neq j} |\langle x_i^{(p)}, x_j^{(p)} \rangle|^p \right)^{1/p} \geq c(X^{(p)}) \geq \mathcal{F}_\infty. \tag{14}$$

On the other hand,

$$\mathcal{F}_p^{1/p} \leq \left(\sum_{i\neq j} |\langle x_i^{(\infty)}, x_j^{(\infty)}\rangle|^p\right)^{1/p} \leq \left(\sum_{i\neq j} \mathcal{F}_\infty^p\right)^{1/p} = \mathcal{F}_\infty[N(N-1)]^{1/p}. \tag{15}$$

Taking the limit of both inequalities gives us the desired limit.

For the second part of the proposition, let $X = \lim_{k\to\infty} X^{(p_k)}$ where $p_k \to \infty$ as $k \to \infty$. Then by (14) and (15),

$$c(X^{(p_k)}) \leq \mathcal{F}_{p_k}^{1/p_k} \leq \mathcal{F}_\infty[N(N-1)]^{1/p_k}.$$

Letting $k \to \infty$, by continuity of the coherence, we get $c(X) \leq \mathcal{F}_\infty$ which forces $c(X) = \mathcal{F}_\infty$. □

Next, we establish a continuity result of $\mathcal{F}_p$.

Proposition 2.3. *The minimal frame potential $\mathcal{F}_p$ is a continuous and non-increasing function of $p \in (0, \infty)$.*

Proof. We first prove that the function is non-increasing. Letting $p > q$, for any $X \in S(N, d)$,

$$\mathrm{FP}_q(X) \geq \mathrm{FP}_p(X) \geq \mathcal{F}_p,$$

so $\mathcal{F}_q = \mathrm{FP}_q(X^{(q)}) \geq \mathcal{F}_p$.

For continuity, we have

$$\sum_{i\neq j, |\langle x_i, x_j\rangle|\neq 0} |\langle x_i, x_j\rangle|^q \ln|\langle x_i, x_j\rangle| \leq \frac{\mathrm{FP}_p(X) - \mathrm{FP}_q(X)}{p-q},$$

which comes from applying the inequality $a^q \ln a \leq \dfrac{a^p - a^q}{p-q}$ for $0 < q < p, a > 0$ to every nonzero term in the frame potential.

So

$$\begin{aligned} 0 &\leq \frac{\mathcal{F}_q - \mathcal{F}_p}{p-q} \\ &= \frac{\mathcal{F}_q - \mathrm{FP}_p(X^{(p)})}{p-q} \\ &\leq \frac{\mathrm{FP}_q(X^{(p)}) - \mathrm{FP}_p(X^{(p)})}{p-q} \\ &\leq \sum_{i\neq j, |\langle x_i^{(p)}, x_j^{(p)}\rangle|\neq 0} |\langle x_i^{(p)}, x_j^{(p)}\rangle|^q \ln\frac{1}{|\langle x_i^{(p)}, x_j^{(p)}\rangle|} \leq \sum_{i\neq j, |\langle x_i^{(p)}, x_j^{(p)}\rangle|\neq 0} \ln\frac{1}{|\langle x_i^{(p)}, x_j^{(p)}\rangle|} := C_p. \end{aligned}$$

Therefore $0 \leq \mathcal{F}_q - \mathcal{F}_p \leq (p-q)C_p$, which implies the continuity of $\mathcal{F}$. □

Next, for fixed p, d, we consider the asymptotics of $\mathcal{F}_{p,N,d}$ as the number of points N grows. In particular, we have that $\mathcal{F}_N \sim N^2$, see Proposition 2.6. We note that this behavior was numerically observed in [1]. Such asymptotic result is standard in the minimal energy literature, and can be found in [16] by Farkas and Nagy in a more general setting. For the sake of completeness, we reproduce their proof below. We begin by establishing some preliminary results.

Lemma 2.4. *Given $d \geq 2$, and $p \in (0, \infty)$, the sequence $\left\{\frac{\mathcal{F}_{p,N}}{N(N-1)}\right\}_{N \geq d+1}$ is a non-decreasing sequence.*

Proof. Let $X^{(N)} = \{x_i^{(N)}\}_{i=1}^N$ be an optimal configuration for $\mathrm{FP}_{p,N,d}$. For each $k \in [1:N]$,

(16)
$$\mathcal{F}_N = \mathrm{FP}(X^{(N)}) = \mathrm{FP}\left(X^{(N)} \backslash \{x_k^{(N)}\}\right) + 2\sum_{j \neq k} |\langle x_k^{(N)}, x_j^{(N)} \rangle|^p \geq \mathcal{F}_{N-1} + 2\sum_{j \neq k} |\langle x_k^{(N)}, x_j^{(N)} \rangle|^p.$$

Summing (16) over k, we obtain

$$N\mathcal{F}_N \geq N\mathcal{F}_{N-1} + 2\mathcal{F}_N \Longrightarrow (N-2)\mathcal{F}_N \geq N\mathcal{F}_{N-1} \Longrightarrow \frac{\mathcal{F}_N}{N(N-1)} \geq \frac{\mathcal{F}_{N-1}}{(N-1)(N-2)}.$$

□

It follows that $\tau := \lim_{N\to\infty} \frac{\mathcal{F}_{p,N}}{N^2}$ exists. In fact, in the minimal energy literature, τ is called the transfinite diameter due to Fekete. Furthermore, τ is related to the continuous version of the frame potential, which is introduced in [15]. More specifically, given a probabilistic measure μ on the sphere, the *probabilistic p frame potential* is defined as

$$\mathrm{PFP}_{p,d}(\mu) := \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} |\langle x, y \rangle|^p d\mu(x) d\mu(y). \tag{17}$$

Let $\mathcal{M}(\mathbb{S}^{d-1})$ be the collection of all probabilistic measures on the sphere. Simple compactness and continuity arguments show that

$$\mathcal{P}_{p,d} := \min_{\mu \in \mathcal{M}(\mathbb{S}^{d-1})} \mathrm{PFP}_{p,d}(\mu) \tag{18}$$

exists.

Given any N point configuration X, its normalized counting measure is defined as

$$\nu_X := \frac{1}{N} \sum_{x \in X} \delta_x.$$

We have

$$\mathrm{PFP}_{p,d}(\nu_X) = \int \int |\langle x, y \rangle|^p d\nu_X(x) d\nu_X(y) = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |\langle x_i, x_j \rangle|^p = \frac{\mathrm{FP}_{p,N,d}(X) + N}{N^2}. \tag{19}$$

Consequently, if X is an optimal configuration, i.e., $\mathcal{F}_{p,N} = \mathrm{FP}_{p,N,d}(X)$, then by (19), it is plausible that $\tau = \mathcal{P}_{p,d}$.

Lemma 2.5. *Given $d \geq 2$ and $p \in (0, \infty)$, $\tau = \lim_{N\to\infty} \dfrac{\mathcal{F}_{p,N,d}}{N^2} \leq \mathcal{P}_{p,d}$.*

Proof. Let μ^* be the optimal probabilistic measure, that is,

$$\int \int |\langle x, y \rangle|^p d\mu^*(x) d\mu^*(y) = \mathcal{P}_{p,d} = \mathrm{PFP}_{p,d}(\mu^*).$$

Consequently,

$$\begin{aligned}\mathcal{F}_{p,N,d} &= \int \cdots \int \left[\min_X \mathrm{FP}(X)\right] d\mu^*(x_1)\cdots d\mu^*(x_N)\\ &\le \int \cdots \int \mathrm{FP}(X) d\mu^*(x_1)\cdots d\mu^*(x_N)\\ &= \sum_{i\neq j} \int \cdots \int |\langle x_i, x_j\rangle|^p d\mu^*(x_1)\cdots d\mu^*(x_N) = \sum_{i\neq j} \mathcal{P}_{p,d} = N(N-1)\mathcal{P}_{p,d}.\end{aligned}$$

The result follows by dividing N^2 on both sides and taking the limit. □

Proposition 2.6. *Given $d \ge 2$ and $p \in (0,\infty)$, we have $\tau = \lim_{N\to\infty} \dfrac{\mathcal{F}_{p,N,d}}{N^2} = \mathcal{P}_{p,d}$. Moreover, if $\{X_N\}_{N\ge d+1}$ is a sequence of N-point configurations such that $\lim_{N\to\infty} \frac{FP_N(X_N)}{N^2} = \tau$, then every weak star cluster point ν^* of the normalized counting measure $\nu_{X_N} = \frac{1}{N}\sum_{x\in X_N}\delta_x$ solves (18), that is $PFP_{p,d}(\nu^*) = \mathcal{P}_{p,d}$. In particular, this holds for any sequence of the optimal configurations of FP_N.*

Proof. By weak star convergence and (19),

$$\mathcal{P}_{p,d} \le \mathrm{PFP}_{p,d}(\nu^*) = \lim_{N\to\infty} \mathrm{PFP}_{p,d}(\nu_{X_N}) = \lim_{N\to\infty} \frac{\mathrm{FP}_{p,N,d}(X_N) + N}{N^2} = \tau.$$

In view of Lemma 2.5, we have $\tau = \mathcal{P}_{p,d}$ and ν^* is an optimal probabilistic measure. □

The exact value of τ can be found in many cases. We list two examples in the following corollary.

Corollary 2.7. *(a) When $d \ge 2$ and $p \in (0,2]$, we have $\lim_{N\to\infty} \dfrac{\mathcal{F}_{p,N,d}}{N^2} = \mathcal{P}_{p,d} = \dfrac{1}{d}$.*

(b) When $d = 2$ and p is an even integer, we have $\lim_{N\to\infty} \dfrac{\mathcal{F}_{p,N,2}}{N^2} = \mathcal{P}_{p,2} = \dfrac{1\cdot 3\cdot 5\cdots(p-1)}{2\cdot 4\cdot 6\cdots p}$.

Proof. (a) By [15, Theorem 3.5] we know that when $N = kd$, the frame potential is minimized by k copies of orthonormal basis. So $\lim_{N\to\infty} \frac{\mathcal{F}_{p,N,d}}{N^2} = \lim_{k\to\infty} \frac{\mathcal{F}_{p,kd,d}}{(kd)^2} = \lim_{k\to\infty} \frac{(k-1)kd}{(kd)^2} = \frac{1}{d}$. Note that this recovers [15, Theorem 4.9], which states that $\mathcal{P}_{p,d} = \frac{1}{d}$.

(b) In dimension $d = 2$, it is known that $2N$ equally spaced points on the unit circle are spherical $(2N-1)$-design ([25, Section 4]), so Proposition 1.1 implies that $X_N^{(h)}$ is an optimal configuration if $p \le 2N-2$ is an even integer. In other words, with fixed even integer p, when N is large enough, $\left(X_N^{(h)}\right)^{sym}$ is going to be a $(2N-1)$-design (hence p-design), so the equality in Proposition 1.1 holds and we get the desired result. □

3. Optimal configurations in dimension 2

This section focuses on the case $d = 2$, when the points are on the unit circle $\mathbb{S}^1 \subset \mathbb{R}^2$.

3.1. **A class of minimal energy problems.** We recall that when $N = 2k$ is even and $0 < p < 2$, the solution to (4) was given in [15, Theorem 3.5], where it was established that the minimizers are k copies of any orthonormal basis of $\mathbb{R}^2$. The case $p = 2$ was settled by

Benedetto and Fickus [3]. In order to address other values of p, we will consider a more general problem

$$\min_{X\subset C_r,|X|=N}\sum_{i\neq j} f(\|x_i-x_j\|^2), \tag{20}$$

where $f:(0,4r^2]\to\mathbb{R}$ is a nonnegative and decreasing function, and C_r is a $1-$dimensional circle with radius r. This circle C_r does not need to be centered at 0 and could be in any dimension. It will become clear later why we require points on a general circle instead of the usual $\mathbb{S}^1$.

The first result only requires f to be convex, but it only works for up to 4 points.

Theorem 3.1. *Given $r>0$, let $f:(0,4r^2]\to\mathbb{R}$ be a decreasing convex function. Any configuration X_4^* of 4 equally spaced points on C_r is an optimal configuration of (20) with $N=4$. If in addition, f is strictly convex, then no other 4-point configuration is optimal.*

Proof. Let $X_4=\{x_i\}_{i=1}^4$ be an arbitrary configuration with x_i ordered counter clockwise. Let $\alpha_{ik}\in[0,2\pi)$ be the angle between x_i and x_{i+k} for any $k\in[1:3]$. The index of the vectors is cyclic as $x_i=x_{i-4}$. Then $\|x_i-x_{i+k}\|^2=2r^2-2r^2\cos\alpha_{ik}=4r^2\sin^2\frac{\alpha_{ik}}{2}$. It is evident that $\sum_{i=1}^4\alpha_{ik}=2\pi k$. Using the convexity of f,

$$\begin{aligned}\sum_{i\neq j} f\big(\|x_i-x_j\|^2\big)&=\sum_{k=1}^3\sum_{i=1}^4 f\big(\|x_i-x_{i+k}\|^2\big)=4\sum_{k=1}^3\frac{1}{4}\sum_{i=1}^4 f\big(\|x_i-x_{i+k}\|^2\big)\\&\geq 4\sum_{k=1}^3 f\left(\frac{1}{4}\sum_{i=1}^4\|x_i-x_{i+k}\|^2\right)=4\sum_{k=1}^3 f\left(\frac{4r^2}{4}\sum_{i=1}^4\sin^2\frac{\alpha_{ik}}{2}\right).\end{aligned} \tag{21}$$

Next, let $\beta_{ik}=\alpha_{ik}/2$. In order to minimize the right hand side of (21), we solve

$$\max\sum_{i=1}^4\sin^2\beta_{ik}\quad\text{subject to}\quad\beta_{ik}\geq 0,\ \sum_{i=1}^4\beta_{ik}=\pi k.$$

When $k=1$, we let $\beta_i=\beta_{i1}$ for short. Using Lagrange multipliers, we have $0=\frac{\partial}{\partial\beta_j}[\sum_{i=1}^4\sin^2\beta_i+\lambda(\sum_{i=1}^4\beta_i-\pi)]=\sin 2\beta_j+\lambda$, which implies that

$$\sin 2\beta_i=\sin 2\beta_j\Longrightarrow 2\beta_i=2\beta_j,\ \text{or}\ 2\beta_i+2\beta_j=\pi,$$

since $\sum_{i=1}^4\beta_i=\pi$.

If we are in the case that $\beta_1+\beta_2=\pi/2$ (or any pair $i\neq j$ with $\beta_i+\beta_j=\pi/2$), then $\sum_{i=1}^4\sin^2\beta_i=\sin^2(\beta_1)+\sin^2(\pi/2-\beta_1)+\sin^2(\beta_3)+\sin^2(\pi/2-\beta_3)=2$. If we are in the other case that $\beta_1=\beta_2=\beta_3=\beta_4$, then $\sum_{i=1}^4\sin^2\beta_i=4\sin^2\frac{\pi}{4}=2$. So for $k=1$,

$$\sum_{i=1}^4\sin^2\beta_{i1}\leq 4\sin^2\frac{\pi}{4},$$

and the equality holds when $\beta_{i1}+\beta_{j1}=\pi/2$ for some $i\neq j$.

When $k=2$, it is obvious that

$$\sum_{i=1}^4\sin^2\beta_{i2}\leq 4=4\sin^2\frac{\pi}{2}$$

with equality at $\beta_{i2}=\pi/2$, for all $i\in[1:4]$. This implies that $\beta_{i1}+\beta_{i+1,1}=\pi/2$ for some i.

When $k=3$, $\sum_{i=1}^4 \sin^2\beta_{i3} = \sum_{i=1}^4 \sin^2(\pi-\beta_{i1}) = \sum_{i=1}^4 \sin^2\beta_{i1}$ which reduces to the $k=1$ case.

In summary, for any $k=1,2,3$,

$$\sum_{i=1}^4 \sin^2\frac{\alpha_{ik}}{2} \le 4\sin^2\frac{\pi k}{4},$$

and the equality holds simultaneously when $\alpha_{i1}+\alpha_{i+1,1}=\pi$, or equivalently $x_1+x_3=0, x_2+x_4=0$.

Following (21), we have

(22)

$$\sum_{i\neq j} f\big(\|x_i-x_j\|^2\big) \ge 4\sum_{k=1}^3 f\Big(\frac{4r^2}{4}\sum_{i=1}^4 \sin^2\frac{\alpha_{ik}}{2}\Big) \ge 4\sum_{k=1}^3 f\Big(4r^2\sin^2\frac{\pi k}{4}\Big) = 8f(2r^2)+4f(4r^2).$$

It is easy to check that four equally spaced points on C_r achieve this minimum.

If f is strictly convex, then the inequality of (21) becomes equality if $\|x_i - x_{i+k}\| = \|x_j - x_{j+k}\|$ for every $i\neq j$, which only holds for equally spaced points. □

Remark 3.2. The proof of Theorem 3.1 breaks down for $N\ge 5$ because $\sum_{i=1}^N \sin^2\beta_{i1}$ is not maximized at equally spaced points.

Our second result regarding (20) is a variation of the main result of the work by Cohn and Kumar [12, Theorem 1.2]. Let m be a positive integer. An *m-sharp configuration* $X\subset\mathbb{S}^{d-1}$ is a spherical $(2m-1)$-design with m inner products between its distinct points. It was proven in [12] that sharp configurations are the unique universal optimal configurations of the problem

$$\min_{X\in S(N,d)} \sum_{i\neq j} f(\|x_i-x_j\|^2), \tag{23}$$

for completely monotonic functions f. A C^∞ function $f: I\to\mathbb{R}$ is called *K-completely monotonic* if $(-1)^k f^{(k)}(x)\ge 0$ for all $x\in I$ and all $k\le K$, and *strictly K-completely monotonic* if strict inequality always holds in the interior of I. The notion ∞-completely monotonic is simply called *completely monotonic* as traditionally defined, which means $(-1)^k f^{(k)}(x)\ge 0$ for all $x\in I$ and all $k\ge 0$. A list of known sharp configurations was given in [12]. For example, N equally spaced points on $\mathbb{S}^1$ is an $\lfloor N/2\rfloor$-sharp configuration.

Another notion that we will need is that of absolutely monotonic functions. A C^∞ function $f: I\to\mathbb{R}$ is called *K-absolutely monotonic* if $f^{(k)}(x)\ge 0$ for all $x\in I$ and all $k\le K$. Similarly, ∞-absolutely monotonic means the inequality is true for all nonnegative integers k, and will be simply referred to as *absolutely monotonic*. It is straightforward that $f(t)$ being completely monotonic is equivalent to $f(-t)$ being absolutely monotonic.

As remarked by [12], the complete monotonicity on f can be weakened slightly. To ensure a good flow of the paper, the proof of the next result which is a variation of [12, Theorem 1.2] will be given in the appendix.

Theorem 3.3. *Fix a positive integer m and let $f:(0,4]\to\mathbb{R}$ be a function such that $(-1)^k f^{(k)}(t)\ge 0$ for all $t\in(0,4], k\le 2m$. Then an m-sharp configuration is an optimal configuration of (23). Furthermore, if $(-1)^k f^{(k)}(t)>0$ for all $t\in(0,4), k\le 2m$, then the m-sharp configuration is the unique optimal configuration of (23).*

A direct consequence of Theorem 3.3 for dimension $d = 2$ is that equally spaced points are optimal configurations if the energy kernel function f is completely monotonic up to certain order. But notice that $\sum_{i\neq j} f(\|x_i - x_j\|^2)$ only depends on the relative distances between x_i's so the result should be true for any circle C_r (whose radius is r) if we rescale f properly.

Corollary 3.4. *For $N \geq 4$, let $m = \lfloor N/2 \rfloor$. For $r > 0$, suppose that $f : (0, 4r^2] \to \mathbb{R}$ is completely monotonic up to $2m$. Then N equally spaced points on C_r is an optimal configuration of (20). Moreover, if f is strictly completely monotonic up to $2m$, then the equally spaced points is the unique optimal configuration of (20).*

3.2. **A lifting trick.** How do Theorem 3.1 and Corollary 3.4 help to solve the frame potential problem? On the unit circle, we have $|\langle x_i, x_j\rangle|^p = \left|\frac{2-\|x_i-x_j\|^2}{2}\right|^p = h(\|x_i - x_j\|^2)$, where $h(t) = \left|\frac{2-t}{2}\right|^p$. Unfortunately neither result can be applied because the function $h(t)$ is not differentiable at $t = 2$ unless p is an even integer; worse, it is not even decreasing on [0,4]. This should not come as a surprise since the frame potential does not distinguish between antipodal points. Consequently, rather than analyzing the frame potential in terms of the distance between vectors, we should consider it in terms of the distance between lines, as was done in [11].

Define $P : \mathbb{S}^{d-1} \to M(d, d)$ as $P(x) = xx^*$, where $M(d, d)$ is the space of $d \times d$ symmetric matrices endowed with the Frobenius norm. $P(\mathbb{S}^{d-1})$ identifies antipodal points, and is the projective space embedded in $M(d, d)$. We write $P(x)$ as P_x and list some of the properties.

$$\begin{cases} \langle P_x, P_y\rangle &= |\langle x, y\rangle|^2 \\ \|P_x - P_y\|^2 &= 2 - 2|\langle x, y\rangle|^2. \end{cases} \tag{24}$$

When $d = 2$, we can explicitly write the embedding as $P : \mathbb{S}^1 \to M(2, 2)(= \mathbb{R}^3)$,

$$P(x) = P_x = xx^* = \begin{bmatrix} x_1^2 & x_1x_2 \\ x_1x_2 & x_2^2 \end{bmatrix} \longleftrightarrow (x_1^2, \sqrt{2}x_1x_2, x_2^2).$$

It is not hard to see that $P(\mathbb{S}^1)$ is a circle in $\mathbb{R}^3$ centered at $(\frac{1}{2}, 0, \frac{1}{2})$ with radius $r = \frac{1}{\sqrt{2}}$, and this is where we can apply Theorem 3.1 or Corollary 3.4. One can verify that equally spaced points on the circle $P(\mathbb{S}^1)$ are precisely $X_N^{(h)}$, equally spaced points on the half circle, so we have the following theorem.

Theorem 3.5. *Let $g : [0, 1) \to \mathbb{R}$ and consider*

$$\min_{X\in S(N,2)} \sum_{i\neq j} g(|\langle x_i, x_j\rangle|^2), \tag{25}$$

Then the following statements hold.

- *(a) If g is convex and increasing, then $X_4^{(h)}$ is an optimal configuration of (25) when $N = 4$. Moreover if g is strictly convex, then $X_4^{(h)}$ is the unique optimal configuration.*
- *(b) If g is absolutely monotone up to $2\lfloor N/2 \rfloor$, then $X_N^{(h)}$ is an optimal configuration of (25). Moreover if g is strictly absolutely monotone up to $2\lfloor N/2 \rfloor$, then $X_N^{(h)}$ is the unique optimal configuration.*

Proof. As defined, $P_{x_i} = x_ix_i^*$. Denote P_{x_i} by P_i for simplicity. By (24),

$$g(|\langle x_i, x_j\rangle|^2) = g(1 - \|P_i - P_j\|^2/2) =: f(\|P_i - P_j\|^2),$$

where $f(t) = g(1 - t/2)$ is defined on $(0, 2]$. As discussed earlier, view the points P_i on a circle in $\mathbb{R}^3$ with radius $1/\sqrt{2}$, so solving (25) is equivalent to solving (20) with $r = 1/\sqrt{2}$.

If g is convex and increasing, then f is convex and decreasing. Applying Theorem 3.1 gives equally spaced P_i, which is equally spaced points on the half circle. This is part (a).

If g is absolutely monotone up to $2\lfloor N/2 \rfloor$, then f is completely monotone up to $2\lfloor N/2 \rfloor$. Applying Corollary 3.4 gives part (b).

□

Remark 3.6. Observe that in Theorem 3.5, the assumption of (b) is much stronger than (a). If g is twice differentiable, then g being convex and decreasing is equivalent to g being absolutely monotone up to 2. Furthermore, Theorem 3.5 is a very general result that goes beyond frame potentials. Indeed, it cover the cases where the energy can be expressed as a function of squares of the inner products. We expect to pursue this line of investigations elsewhere, with the goal of analyzing other energy kernels suitable for finding certain well conditioned frames.

Finally we are ready to state the promised frame potential result as a special case of Theorem 3.5.

Theorem 3.7. *Let $X_N^{(h)}$ be the equally spaced points on half of the circle $\mathbb{S}^1$ as in* (10)*. The following statements hold.*

(a) If $N = 4$ and $p > 2$, then $X_4^{(h)}$ is the unique optimal configuration of (4)*.*

(b) If $N \geq 5$ and $p > \begin{cases} 2N-2, & N \text{ is even} \\ 2N-4, & N \text{ is odd} \end{cases}$, then $X_N^{(h)}$ is the unique optimal configuration of (4)*.*

(c) If $N \geq 5$, and $2 < p \leq \begin{cases} 2N-2, & N \text{ is even} \\ 2N-4, & N \text{ is odd} \end{cases}$ is an even integer, then $X_N^{(h)}$ is an optimal configuration of (4)*, but it is unclear whether there are other optimal configurations.*

Proof. The p-frame potential kernel $|\langle x_i, x_j \rangle|^p = g_p(|\langle x_i, x_j \rangle|^2)$ with $g_p(t) = t^{p/2}$. The function g_p is strictly convex and increasing on [0,1) if $p > 2$.

(a) This part is due to Theorem 3.5(a).

(b) We notice that g_p is strictly absolutely monotone up to $\lceil p/2 \rceil$, where $\lceil c \rceil$ is the smallest integer that is no less than c. In order to apply Theorem 3.5(b), we require $\lceil p/2 \rceil \geq 2\lfloor N/2 \rfloor$, which is equivalent to $p > 2N - 2$ if N is even and $p > 2N - 4$ if N is odd.

(c) Finally, this part is true because g_p is absolutely monotone when p is an even integer.

□

Remark 3.8. By Proposition 2.6, we can let p go to infinity in Theorem 3.7 and get that $X_N^{(h)}$ is the Grassmannian frame, as was shown in [5].

As seen, the 1-dimensional projective space is isomorphic to a circle. It is well known that higher a dimensional projective space is not a higher dimensional sphere. This is why the main result Theorem 3.5 is limited to $d = 2$.

At this point, we summarize the p-frame potential results in $\mathbb{S}^1$ as the following remark.

Remark 3.9. Let $d = 2$.

(a) When $N = 4$ we have completed the characterization of $\mathcal{F}_{p,4,2}$.
(b) When $N \geq 6$ is even, then [15, Theorem 3.5] and parts (b) and (c) of Theorem 3.7 give the value of $\mathcal{F}_{p,N,2}$ when $p \in (0,2] \cup \{4, 6, \cdots, 2N-2\} \cup (2N-2, \infty)$. We further know that the minimizer is unique for $p \in (0,2) \cup (2N-2, \infty)$. It is still open for $p \in (2, 2N-2]$ though we expect $X_N^{(h)}$ to be a minimizer. The numerical result is displayed in Figure 1 for $N = 6$.
(c) When $N \geq 5$ is odd, we know $\mathcal{F}_{p,N,2}$ for $p \in \{2, 4, \cdots, 2N-4\} \cup (2N-4, \infty)$. We suspect that for $p \in (2, 2N-4]$, $X_N^{(h)}$ will still be the minimizer. The case $p \in (0,2)$ seems rather intriguing as demonstrated in Figure 1 for $N = 5$.

Figure 1 displays the numerical experiment for $d = 2$ and $N = 5, 6$. According to the numerical experiment, $\mathcal{F}_{p,6,2}$ is achieved by $X_6^{(h)}$ for $p \in (2, 10]$. The $N = 5$ case is more complex. It appears that for p from 0 to about 1.78, the optimal configuration is two copies of ONB plus a repeated vector; for $p \in (1.78, 2)$, the optimal configuration has the structure $\{x, x, y, y, z\}$ whose angles vary as p changes; for $p \in (2, 6)$, the optimal configuration is $X_5^{(h)}$

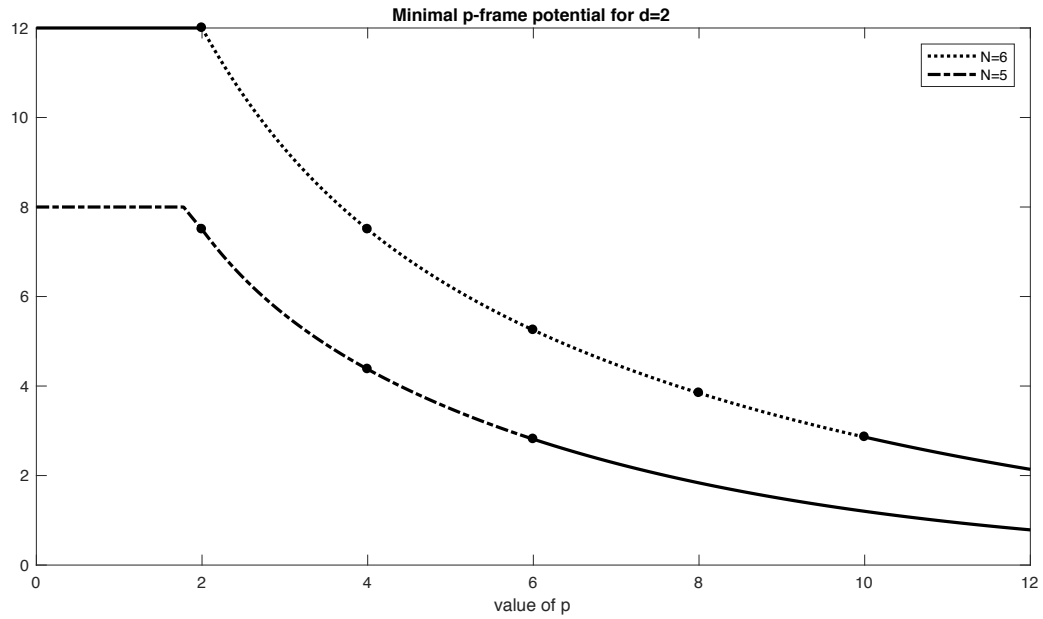

FIGURE 1. The top curve represents $\mathcal{F}_{p,6,2}$ while the lower one represents $\mathcal{F}_{p,5,2}$. The solid portion indicates proven cases as commented in Remark 3.9.

4. Special case of $N = d + 1$ points in dimension d.

In this last section, we report on some numerical experiments and the resulting conjectures when minimizing the p-frame potential with $N = d+1$ vectors in $\mathbb{R}^d$, and $p \in (0, \infty)$. Observe that the case $p = 2$ is a special case of the work by Benedetto and Fickus [3]. Additionally, the case $p > 2$ is handled by Ehler and Okoudjou [15, Proposition 3.1], for which the simplex is the optimal configuration. To be specific, the simplex is an ETF of $d + 1$ vectors for $\mathbb{R}^d$. Therefore, the focus in this section are values $p < 2$. The following definition will be used through the rest of this section.

Definition 4.1.

(a) X is an ONB+ if X is formed by an orthonormal basis of $\mathbb{R}^d$ with one of the vectors repeated.
(b) Given $n \geq 2$, the simplex of $\mathbb{R}^n$ is denoted by ETF_n. An explicit construction of ETF_n is to project $e_1, e_2, \cdots, e_n, e_{n+1}$, the canonical basis of $\mathbb{R}^{n+1}$, onto the orthogonal complement of $\sum_{i=1}^{n+1} e_i$.

4.1. **Embedded ETFs.** From numerical tests, we have noticed that minimizers for $\mathcal{F}_{p,d+1,d}$ take forms similar to ETFs. In particular, they take the form of ETFs that have been embedded to higher dimensions.

Definition 4.2. For $1 \leq k \leq d$, the frame

$$\mathrm{L}_k^d = \begin{bmatrix} \mathrm{ETF}_k & 0 \\ 0 & I_{d-k} \end{bmatrix} = \begin{bmatrix} \mathrm{ETF}_k & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \in S(d+1, d)$$

is called an *embedded ETF*.

Remark 4.3.

(a) The L_k^d frames are not tight, except for the case $k = d$, and we have L_d^d is ETF_d.
(b) In addition to considering ETF_d as an L_d^d configuration, ONB+ is the L_1^d frame.

Example 4.4. The ETF in $\mathbb{R}^2$ can be embedded to $\mathbb{R}^3$ as

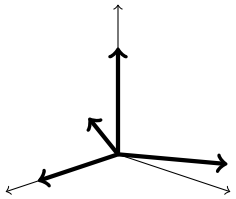

FIGURE 2. The L_2^3 frame

$$\mathrm{L}_2^3 = \begin{bmatrix} 1 & -1/2 & -1/2 & 0 \\ 0 & \sqrt{3}/2 & -\sqrt{3}/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

We see that this frame is neither tight nor equiangular by computing the frame operator and Grammian,

$$S = \begin{bmatrix} 3/2 & 0 & 0 \\ 0 & 3/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad G = \begin{bmatrix} 1 & -1/2 & -1/2 & 0 \\ -1/2 & 1 & -1/2 & 0 \\ -1/2 & -1/2 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

More generally, the Grammian of the L_k^d frame is

$$\begin{bmatrix} 1 & -1/k & -1/k & \cdots & -1/k & 0 & 0 & \cdots & 0 \\ -1/k & 1 & -1/k & \cdots & -1/k & 0 & 0 & \cdots & 0 \\ -1/k & -1/k & 1 & \cdots & -1/k & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1/k & -1/k & -1/k & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \tag{26}$$

indicating that each L_k^d frame is a two-distance set (see [14, 2]) with inner products $-1/k$ and 0; note, however, that L_d^d, or the ETF_d configuration, will have only one inner product, $-1/d$.

4.2. **Embedded ETFs as the Conjectured Minimizers.** Numerical computations suggest that the L_k^d frames are minimizers of $\mathrm{FP}_{p,d+1,d}$.

Conjecture 4.5. *Suppose $d \geq 2$ and for every natural number $1 \leq k \leq d-1$, let*

$$p_k = \frac{\log(k+2) - \log k}{\log(k+1) - \log k}.$$

We also define $p_0 = 0$. The following configurations minimize the p-frame potential $FP_{p,d+1,d}$:

- *when $p \in (p_{k-1}, p_k]$, the L_k^d configuration, $k = 1, 2, \cdots, d-1$;*
- *when $p \in (p_{d-1}, \infty]$, the ETF_d, or L_d^d configuration.*

Certain cases have been known for some time. The case $d = 2$ is completely established in [15]. For $d \geq 3$, the statement that ETF_d is the minimizer follows from [3] when $p = 2$, from [15, Proposition 3.1] when $p > 2$, and from [23] for $p = \infty$. A. Glazyrin [17] recently established that the ONB+, or L_1^d is the optimal configuration for $p \in (0, 2(\frac{\ln 3}{\ln 2} - 1)]$, leading to the fact that $\mathcal{F}_{p,d+1,d} = 2$ for all p in this range and all $d \geq 2$. The number $2(\frac{\ln 3}{\ln 2} - 1)$ is approximately 1.17 and is less than p_1. While revising this manuscript we became aware of the work by Zhiqiang Xu and Zili Xu [27], where they prove the rest of the conjecture. Figure 3 visualizes this conjecture prior to the work [27].

The values p_k may be found by using the p-frame potentials of the L_k^d frames. By (26),

$$\mathrm{FP}_{p,d+1,d}(\mathrm{L}_k^d) = \big((k+1)^2 - (k+1)\big)\left(\frac{1}{k}\right)^p = (k+1)k\left(\frac{1}{k}\right)^p.$$

We find p_k so that the p-frame potentials of L_k^d and L_{k+1}^d are equal at the value p_k, so

$$(k+1)k\left(\frac{1}{k}\right)^{p_k} = (k+2)(k+1)\left(\frac{1}{k+1}\right)^{p_k}$$

leads to $p_k = \frac{\log(k+2)-\log k}{\log(k+1)-\log k}$.

Remark 4.6.

(a) The value p_k, where the p-frame potential of the L_{k+1}^d frame drops below the p-frame potential of the L_k^d frame, does not depend on d, the overall dimension.

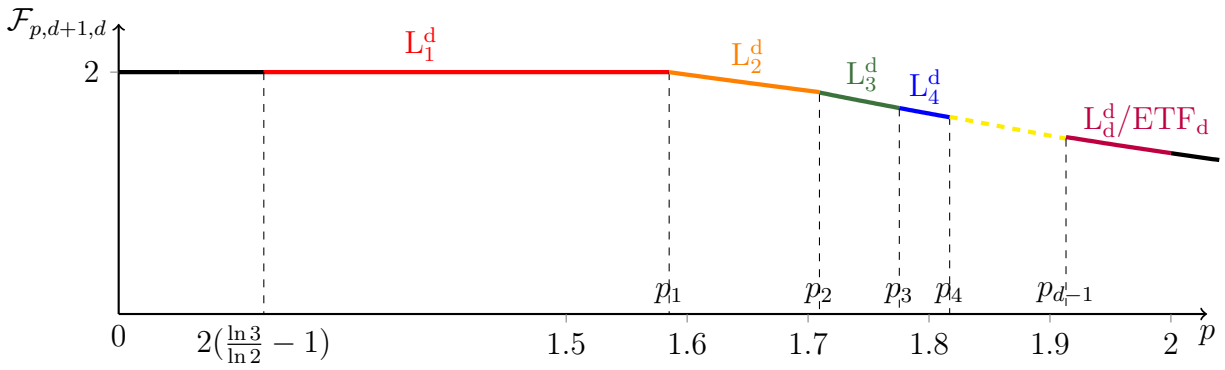

FIGURE 3. Optimal configurations for $\mathcal{F}_{p,d+1,d}$ as p increases from 0 to ∞ according to Conjecture 4.5. The black lines are cases proven before [27].

(b) Following Conjecture 4.5, we will call the values p_k the *switching points* as these are the values of p where the minimizing configuration seems to change. The final switching point is approaching to 2:

$$\lim_{d\to\infty} p_{d-1} = \lim_{d\to\infty} \frac{\log\left(\frac{d+1}{d-1}\right)}{\log\left(\frac{d}{d-1}\right)} = 2.$$

4.3. **Description of the Numerical Computations.** Numerical computations in Sage [24] were used to test Conjecture 4.5 numerically for $d+1$ vectors in $\mathbb{R}^d$. For each $d = 3,4,5,6,7$ and each $k = 1,2,\dots,d$, the program checked numerically whether L_k^d is the minimizer on the regions $[p_{k-1}, p_k]$. For $p = p_{k-1}$ and for $p = p_k$ specifically, along with some random values p in $[p_{k-1}, p_k]$, it used a basic gradient descent to numerically minimize the p-frame potential of several randomly chosen frames and then it compared these to the appropriate L_k^d frame. The only lower frame potential found seemed within the realm of numerical error (`<1e-15`). The number of comparisons was not selected rigorously; rather we only use the program as a guide. More details and the code may be found online at `https://www.math.umd.edu/~okoudjou/`.

5. Appendix: Proof of Theorem 3.3

We now give a proof of Theorem 3.3. Let f be a smooth function. Given a polynomial g with $\deg(g) \geq 1$, let $H(f,g)$ denote the Hermite interpolating polynomial of degree less than $\deg(g)$ that agrees with f at each root of g to the order of that root. The following fact is proven in the proof of [12, Proposition 2.2].

Lemma 5.1. *Let a be differentiable up to K on a subset of $[-1,1)$, and g_1, g_2 be two polynomials such that $\deg(g_1) + \deg(g_2) \leq K$, then $H(a, g_1g_2) = H(a,g_1) + g_1 H(Q(a,g_1), g_2)$ where*

$$Q(a,g) := \frac{a - H(a,g)}{g}.$$

We provide a variation of [12, Proposition 2.2] below. The proof is also similar.

Proposition 5.2. *Let $c, d \in \mathbb{R}$. If a is (strictly) K-absolutely monotone on (c,d), then given any nonconstant polynomial g, $Q(a,g) = \frac{a-H(a,g)}{g}$ is (strictly) absolutely monotone up to $K - \deg g$ on (c,d).*

Proof. By [12, Lemma 2.1],

$$Q(a,g)(t) = \frac{a(t) - H(a,g)(t)}{g(t)} = \frac{a^{(\deg g)}(\xi)}{\deg g!} \tag{27}$$

for some $\xi \in (c,d)$.

A direct consequence of Lemma 5.1 is that $Q(a, g_1g_2) = Q(Q(a,g_1),g_2)$. For $n \in [1 : K - \deg(g)]$, $s_0 \in (c,d)$, there exists $\xi' \in (c,d)$ such that

$$\frac{Q(a,g)^{(n)}(s_0)}{n!} = Q\left(Q(a,g),(t-s_0)^n\right)(s_0) = Q(a,(t-s_0)^n g)(s_0) = \frac{a^{(n+\deg g)}(\xi')}{(n+\deg g)!}. \tag{28}$$

The right hand side of (28) is nonnegative due to the absolute monotonicity of a. □

We also need to define a different version of conductivity here.

Definition 5.3. A nonconstant polynomial g with all its roots in $[-1,1)$ is *K-conductive* if for any K-absolutely monotone function a on $[-1,1)$, $H(a,g)$ is positive definite.

The following Lemma is a variation of [12, Lemma 5.3].

Lemma 5.4. *If g_1 and g_2 are K-conductive and g_1 is positive definite, then g_1g_2 is $(K + \deg g_1)$-conductive.*

Proof. Let a be $(K + \deg g_1)$-absolutely monotone, then $Q(a,g_1)$ is K-absolutely monotone according to Proposition 5.2. Consequently, $H(Q(a,g_1),g_2)$ is positive definite due to the conductivity of g_2. Finally, $H(a,g_1g_2) = H(a,g_1) + g_1H(Q(a,g_1),g_2)$ is positive definite because all three functions are positive definite and positive definite functions are closed under taking products. □

Proof of Theorem 3.3. Let $-1 \le t_1 < t_2 < \cdots < t_m < 1$ be the m distinct inner products of the m-sharp configuration.

Let $a(t) = f(2-2t)$ be defined on $[-1,1)$ and $h(t)$ be the Hermite interpolating polynomial that agrees with $a(t)$ to order 2 at each t_i (i.e. $h(t_i) = a(t_i)$ and $h'(t_i) = a'(t_i)$). Then using our notation, $h = H(a,F^2)$ where $F = \prod_{i=1}^m (t-t_i)$.

For $r \in [-1,1)$, $l(t) = t - r$ is K-conductive for any $K \ge 0$ since $H(a,l)$ is the nonconstant polynomial $a(r)$. It is also proven in [12, Section 5] that $\prod_{i=1}^j (t-t_i)$ is strictly positive definite for all $j \le m$.

For any $K \ge 0$, $g_1 = t - t_1, g_2 = t - t_2$ are both K-conductive and g_1 is positive definite, then Lemma 5.4 implies that g_1g_2 is $(K+1)$-conductive. Using Lemma 5.4 repeatedly on $g_1 = t - t_j, g_2 = \prod_{i=1}^{j-1}(t-t_i)$, we get that F^2 is K-conductive for any $K \ge 2m$. In particular F^2 is $2m$-conductive and it follows that $h = H(a,F^2)$ is positive definite.

It is also clear that $h(t) \le a(t)$ by applying (27) with $g = F^2$. By [12, Proposition 4.1], the energy has a lower bound that is achieved by the m-sharp configuration.

If further f is strictly $2m$-completely monotone, the uniqueness is the same as in [12, Section 6] where only $a^{(\deg h+1)}(t) > 0$ is needed. This is true since $\deg h + 1 \le 2m$.

□

Acknowledgements

This work was partially supported by the NSF REU grant DMS1359307 at the University of Maryland, College Park. The authors are thankful to Alan Bangura, Michael Dworken, Meghana Raja, Rosemary Smith, Hetian Wu, and Ran Zhang who have partially worked

on the project as participants to the MAPS-REU at the University of Maryland. They would also like to thank, Henry Cohn, Dmitriy Bilyk, Alexey Glazyrin, Matt Guay, Paul Koprowski, Dustin Mixon, Shayne Waldron, and Wei-Hsuan Yu for fruitful discussions. K. A. O. was partially supported by a grant from the Simons Foundation #319197, the U. S. Army Research Office grant W911NF1610008, the National Science Foundation grant DMS 1814253, and an MLK visiting professorship at MIT. We would also like to thank the anonymous reviewers for their comments which help improve the manuscript.

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