



Maximizing expected powers of the angle between pairs of points in projective space

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Abstract

Among probability measures on d -dimensional real projective space, one which maximizes the expected angle $\arccos(\frac{x}{|x|} \cdot \frac{y}{|y|})$ between independently drawn projective points x and y was conjectured to equidistribute its mass over the standard Euclidean basis $\{e_0, e_1, \dots, e_d\}$ by Fejes Tóth (Acta Math Acad Sci Hung 10:13–19, 1959. <https://doi.org/10.1007/BF02063286>). If true, this conjecture evidently implies the same measure maximizes the expectation of $\arccos^\alpha(\frac{x}{|x|} \cdot \frac{y}{|y|})$ for any exponent $\alpha > 1$. The kernel $\arccos^\alpha(\frac{x}{|x|} \cdot \frac{y}{|y|})$ represents the objective of an infinite-dimensional quadratic program. We verify discrete and continuous versions of this milder conjecture in a non-empty range $\alpha > \alpha_{\Delta^d} \geq 1$, and establish uniqueness of the resulting maximizer $\hat{\mu}$ up to rotation. We show $\hat{\mu}$ no longer maximizes when $\alpha < \alpha_{\Delta^d}$. At the endpoint $\alpha = \alpha_{\Delta^d}$ of this range, we show another maximizer μ must also exist which is not a rotation of $\hat{\mu}$. For the continuous version of the conjecture, an “Appendix A” provided by Bilyk et al in response to an earlier draft of this work combines with the present improvements to yield $\alpha_{\Delta^d} < 2$. The original conjecture $\alpha_{\Delta^d} = 1$ remains open (unless $d = 1$). However, in the maximum possible range $\alpha > 1$, we show $\hat{\mu}$ and its rotations maximize the aforementioned expectation uniquely on a sufficiently small ball in the L^∞ -Kantorovich–Rubinstein–Wasserstein metric d_∞ from optimal transportation; the same is true for any measure μ which is mutually absolutely continuous with respect to $\hat{\mu}$, but the size of the ball depends on α , d , and $\|\frac{d\hat{\mu}}{d\mu}\|_\infty$.

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1 Introduction

Our previous work explored the embedding of versions of a conjecture by L. Fejes Tóth into one-parameter families of maximization problems parameterized by an exponent $\alpha \in \mathbf{R}$ [18]. As the parameter is varied, the maximizer in each family might theoretically bifurcate continuously or discontinuously, as caricatured by the following elementary examples: for $f_\lambda(x) = -\frac{1}{4}x^4 - \frac{\lambda}{2}x^2$ the maximizer $x_\lambda \in \operatorname{argmax}_{\mathbf{R}} f_\lambda$ bifurcates continuously at $\lambda = 0$ (in a so-called pitchfork), whereas for $f_\lambda(x) = -\frac{1}{4}(1-x^2)^2 - \lambda x$ the maximizer changes discontinuously from $x_\lambda \sim -1$ to $x_\lambda \sim +1$ as λ increases through 0. In the current manuscript, we establish existence and finiteness of a critical threshold for the exponent α in each family, at which our maximizer changes discontinuously unless the corresponding Fejes Tóth conjecture is true. An “Appendix A” by Bilyk, Glazyrin, Matzke, Park, and Vlasiuk leads to an effective bound for the critical threshold in the most symmetrical of these families.

Choose N unoriented lines through the origin of \mathbf{R}^{d+1} . Suppose each pair of lines repel each other with a force whose strength is independent of the (acute) angle between them, so that they prefer to be orthogonal to each other. However, unless $N \leq d+1$, it is impossible for all pairs of lines to be orthogonal. What then are their stable configurations? This question is partly addressed by an unsolved conjecture, which for $d = 2$ dates back to Fejes Tóth [14]: namely that the sum of the angles between these lines is maximized if the lines are distributed as evenly as possible amongst the coordinate axes of some orthonormal basis for \mathbf{R}^{d+1} . For $d \geq 2$ this conjecture has motivated a recent series of works by Bilyk, Dai, Glazyrin, Matzke, Park, Vlasiuk in different combinations [5,7–9], and by Fodor et al. [15]. Other authors have also considered versions of the problem for oriented as well as unoriented lines, in the limit $N = \infty$ —where it can be formulated as an infinite-dimensional quadratic program—and/or with different powers α of the angle or distance between them, e.g. [2,6,11,21]. In recent work we verified the unoriented conjecture for bounded and unbounded values of N in the mild repulsion limit $\alpha = \infty$ [18]. In the present manuscript we shall show there are threshold exponents $\alpha_{\Delta^d}(N) \in [0, \infty)$ and $\alpha_{\Delta^d} = \alpha_{\Delta^d}(\infty) \in [1, \infty)$, such that the same configurations continue to be optimal precisely when $\alpha \geq \alpha_{\Delta^d}(N)$, and uniquely optimal apart from known symmetries if and only if $\alpha > \alpha_{\Delta^d}(N)$. An “Appendix A” provided by Bilyk et al in response to an earlier draft of this work combines with the present improvements to imply $\alpha_{\Delta^d}(N) = \alpha_{\Delta^d} < 2$ for all $d \in \mathbf{N}$ and N divisible by $d+1$, but the conjectured values $\alpha_{\Delta^d} = 1 = \alpha_{\Delta^d}(N)$ for all $N > d+1$ remain open unless $d = 1$. However, we show the same configuration with

arbitrary positive weights remains *locally* optimal—and hence stable—in a suitable sense over the maximal range $\alpha > 1$.

Such explicit characterizations of optimizers which display symmetry breaking are rare in the context of infinite-dimensional quadratic programming, and potentially valuable. In modern data sciences it has also become more and more important to study optimization problems in the curved geometries which arise from dimensional reduction, and we hope our approach to this model problem may also prove relevant in such settings.

The Euclidean unit sphere $\mathbf{S}^d = \{x \in \mathbf{R}^{d+1} \mid |x| = 1\}$ gives a double cover for the real projective space $\mathbf{RP}^d := \mathbf{S}^d / \{\pm\}$ with covering map $x \rightarrow \tilde{x} := \{x, -x\}$. Let ρ be the geodesic distance $\rho(x, y) = \arccos(x \cdot y)$ on \mathbf{S}^d . Define $\Lambda_0 : [0, \pi] \rightarrow \mathbf{R}$ and $\Lambda : \mathbf{S}^d \times \mathbf{S}^d \rightarrow \mathbf{R}$ by

$$\Lambda_0(t) := \frac{2}{\pi} \min\{t, \pi - t\} \quad (1.1)$$

$$\Lambda(x, y) := \Lambda_0(\rho(x, y)), \quad (1.2)$$

so that $\Lambda(x, y)$ is the distance on projective space, rescaled to have unit diameter. Note $\Lambda(x, y) = 1$ if and only if $x \cdot y = 0$.

Let $\mathcal{M}(\mathbf{S}^d)$ denote the set of signed Borel measures on \mathbf{S}^d with finite total variation and $\mathcal{P}(\mathbf{S}^d) := \{0 \leq \mu \in \mathcal{M}(\mathbf{S}^d) \mid \mu(\mathbf{S}^d) = 1\}$ the subset of probability measures. Let $\text{spt}(\mu)$ denote the smallest closed subset of \mathbf{S}^d containing the full mass of μ . For $\alpha > 0$ define the bilinear form

$$B_\alpha(\mu, \nu) := \iint \Lambda^\alpha(x, y) d\mu(x) d\nu(y), \quad \mu, \nu \in \mathcal{M}(\mathbf{S}^d), \quad (1.3)$$

and the corresponding energy

$$E_\alpha(\mu) := \frac{1}{2} B_\alpha(\mu, \mu) \quad \alpha \in (0, \infty]. \quad (1.4)$$

In particular, notice $\Lambda^\infty(x, y) = 1$ if $x \cdot y = 0$, and zero otherwise.

For some $1 \leq \alpha_{\Delta^d} < 2$, we shall establish

$$\max_{\mu \in \mathcal{P}(\mathbf{S}^d)} E_\alpha(\mu) = \frac{d}{2d+2} \text{ if and only if } \alpha \geq \alpha_{\Delta^d}, \quad (1.5)$$

and describe the set of maximizers precisely in the interior $\alpha > \alpha_{\Delta^d}$ of this range.

Write $\mu \equiv \nu$, and say the measures $\mu, \nu \in \mathcal{P}(\mathbf{S}^d)$ are *essentially equivalent*, if and only if there is a rotation $M \in SO(d)$ such that $\mu(A \cup -A) = \nu(M(A \cup -A))$ for each open set $A \subset \mathbf{S}^d$. In other words, $\mu \equiv \nu$ if and only if their canonical projections onto \mathbf{RP}^d are rotations of each other. When a maximum over measures is attained uniquely up to essential equivalence, we say the maximizer is *essentially unique*.

For $N \in \mathbf{N} := \{1, 2, \dots\}$ consider the following collections of discrete probability measures on the d -sphere:

$$\mathcal{P}_N^-(\mathbf{S}^d) := \{\mu \in \mathcal{P}(\mathbf{S}^d) \mid \mu = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}, \quad x_i \in \mathbf{S}^d\},$$

$$\begin{aligned}
\mathcal{P}_{\text{on}}(\mathbf{S}^d) &:= \{\mu \in \mathcal{P}(\mathbf{S}^d) \mid \text{spt}(\mu) \text{ is an orthonormal basis of } \mathbf{R}^{d+1}\}, \\
\mathcal{P}_{\text{on}}^-(\mathbf{S}^d) &:= \{\mu \in \mathcal{P}_{\text{on}}(\mathbf{S}^d) \mid \mu[\{x\}] = \frac{1}{d+1} \quad \forall x \in \text{spt } \mu\}, \\
\mathcal{P}_{\Delta}(\mathbf{S}^d) &:= \{\mu \in \mathcal{P}(\mathbf{S}^d) \mid \mu \equiv \nu \text{ for some } \nu \in \mathcal{P}_{\text{on}}(\mathbf{S}^d)\}, \\
\mathcal{P}_{\Delta}^-(\mathbf{S}^d) &:= \{\mu \in \mathcal{P}(\mathbf{S}^d) \mid \mu \equiv \nu \text{ for some } \nu \in \mathcal{P}_{\text{on}}^-(\mathbf{S}^d)\}.
\end{aligned}$$

The closure $\overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}$ of $\mathcal{P}_{\Delta}(\mathbf{S}^d)$ in the narrow topology denotes the set of measures whose projective support is contained in an orthonormal basis $V = \{v_0, \dots, v_d\}$ —which we think of as forming the vertices of a maximal projective simplex—and $\mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ is the subset of measures which equidistribute their mass over these vertices.

Motivated by [18], the following elementary lemma is our starting point: it establishes existence of a threshold for the transition that we intend to describe:

Lemma 1.1 (Threshold exponent for equidistribution over maximal simplices) *There exists a unique $\alpha_{\Delta^d} \in [1, \infty]$ such that $0 < \alpha < \alpha_{\Delta^d}$ implies $\mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ disjoint from $\text{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha}$, whereas $\alpha_{\Delta^d} < \alpha$ implies*

$$\mathcal{P}_{\Delta}^-(\mathbf{S}^d) = \text{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha}. \quad (1.6)$$

Moreover, (1.6) fails when $\alpha = 1$, meaning $\mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ is either strictly contained in or disjoint from $\text{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_1$.

Proof Fix $0 < \alpha_0 < \infty$. Notice $\Lambda(x, y) \leq 1$ on $\mathbf{S}^d \times \mathbf{S}^d$, with equality if and only if $x \cdot y = 0$. For each $\mu \in \mathcal{P}(\mathbf{S}^d)$, it follows that $\alpha \in (0, \infty] \mapsto E_{\alpha}(\mu)$ is nonincreasing; moreover, it decreases strictly unless each distinct pair of points $x \neq y$ in $\text{spt } \mu$ are orthogonal, i.e. unless $\mu \in \overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}$. On $\overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}$ it is well-known [18] and easy to check

$$\mathcal{P}_{\Delta}^-(\mathbf{S}^d) = \text{argmax}_{\mu \in \overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}} E_{\alpha_0}(\mu) \quad (1.7)$$

using, e.g. the Perron-Frobenius theorem.

Now suppose some (and hence all) $\hat{\mu} \in \mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ attain the maximum (1.5) when $\alpha = \alpha_0$. For $\alpha > \alpha_0$ and $\mu \in \mathcal{P}(\mathbf{S}^d)$, the monotonicity mentioned above implies $E_{\alpha}(\mu) \leq E_{\alpha_0}(\mu) \leq E_{\alpha_0}(\hat{\mu}) = E_{\alpha}(\hat{\mu})$. The first inequality is strict unless $\mu \in \overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}$; for $\mu \in \overline{\mathcal{P}_{\Delta}(\mathbf{S}^d)}$, the second inequality becomes strict unless $\mu \in \mathcal{P}_{\Delta}^-(\mathbf{S}^d)$, according to (1.7). Thus we conclude (1.6) for all $\alpha > \alpha_0$. Taking the infimum of such α_0 yields α_{Δ^d} , with the usual convention $\alpha_{\Delta^d} = \infty$ if no such α_0 exists.

It remains to show $\alpha_{\Delta^d} \geq 1$. When $d = 1$ the energy $E_1(\mu)$ takes the constant value $1/4$ on the closed convex hull of $\mathcal{P}_{\Delta}^-(\mathbf{S}^1)$ —which consists of all measures on $\mathbf{S}^1/\{\pm\}$ that are invariant under a rotation by angle $\pi/2$ —thus includes not only $\hat{\mu}$ but also the uniform measure on \mathbf{S}^1 .

For $d > 1$, it therefore follows that $E_1(\hat{\mu}) = E_1(\mu)$, where $\hat{\mu} = \frac{1}{d+1} \sum_{i=0}^d \delta_{v_i} \in \mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ and μ represents the average of $\hat{\mu}$ with any (or all) of its rotations in the plane spanned by v_0 and v_1 , say. This shows (1.6) cannot hold when $\alpha = 1$, hence $\alpha_{\Delta^d} \geq 1$ as desired. \square

We call the assertion $\alpha_{\Delta^d} = 1$ (regardless of dimension d) the *continuous Fejes Tóth conjecture*, which has remained open at least since 1959 [14], except for one dimension $d = 1$.

A major goal of the present manuscript is to show that at this threshold exponent provided by Lemma 1.1 the inclusion

$$\mathcal{P}_{\Delta}^-(\mathbf{S}^d) \subset \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha_{\Delta^d}} \quad (1.8)$$

becomes strict (Theorem 3.6), meaning the optimizer is no longer essentially unique. For $\alpha_{\Delta^d} < \infty$, the inclusion follows from Γ -convergence ideas explained in Sect. 3; however, its strictness requires us to first establish a new local stability result: Theorem 2.4. This local stability holds in the maximum possible range $\alpha > 1$, thus is consistent with the conjectured value $\alpha_{\Delta^d} = 1$; when combined with the finiteness of α_{Δ^d} shown subsequently it implies discontinuous dependence of the maximizer on α at $\alpha_{\Delta^d} > 1$ otherwise (Corollary 2.6).

When $\alpha = \infty$, the essential unique characterization (1.6) of the optimizer follows from our earlier works [18,19] together with an estimate $N(d)$ on the cardinality of support of local energy maximizers for $\alpha \geq 4$ which develops from the ideas of various authors [13,16,24]. The local stability result established hereafter then implies $\alpha_{\Delta^d} < \infty$. Following our announcement of this result, Bilyk et al reported to us an elegant majorization argument that immediately gives $\alpha_{\Delta^d} \leq 2$; they have kindly agreed to include their argument in the present paper in the form of a separately authored appendix. Motivated in part by this development, we have refined our local stability analysis below to imply $\alpha_{\Delta^d} < 2$. Indeed, for every $\alpha > 1$, our stability analysis now shows each measure in the broader class $\mathcal{P}_{\Delta}(\mathbf{S}^d)$ of unbalanced simplices is an essentially unique local maximizer for the energy $E_{\alpha}(\mu)$ on an appropriately metrized version of the landscape $\mathcal{P}(\mathbf{S}^d)$. To formulate both this stability result (Theorem 2.4) and the Γ -convergence statement for the family of energies $(E_{\alpha})_{\alpha>0}$ requires us to recall the metrics $\{d_p\}_{p \in [1,\infty]}$ on this landscape from the theory of optimal transportation which we use to define the relevant topologies. Unless the conjecture $\alpha_{\Delta^d} = 1$ holds, we show (i) the d_{∞} -continuity of any curve $(\mu_{\alpha})_{\alpha>0}$ of optimizers

$$\mu_{\alpha} \in \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha}$$

must fail at $\alpha = \alpha_{\Delta^d}$ (Corollary 2.6), and (ii) when $\alpha = \alpha_{\Delta^d}$ the optimizers form a disconnected set in the d_{∞} -topology (Corollary 3.9).

These theorems partly echo our results concerning particles interacting via strongly attractive / mildly repulsive potentials on Euclidean space [17]. In the present context, the interaction kernel Λ^{α} acts purely repulsively on \mathbf{RP}^d (or attractive-repulsively on \mathbf{S}^d), with compactness of the space substituting for strong attraction at large distances. The restriction $\alpha \geq 2$ corresponds to the mildly repulsive range of potentials from [3,13,17]. A remarkable difference between our results and those of the Euclidean setting, however, is that the characterization of the optimizers (1.6) continues to hold in the interval $\alpha \in (\alpha_{\Delta^d}, 2) \neq \emptyset$. This helped motivate our effort to exclude the case of equality from the estimate $\alpha_{\Delta^d} \leq 2$ provided by Bilyk et al's appendix. By

contrast, for the analogous problem on Euclidean space, in which the charges interact to minimize the attractive-repulsive pair potential $W(x) = \phi(x) - \frac{1}{\alpha}|x|^\alpha$, Balagué et al [3] have shown that, e.g., $\phi \in C_{loc}^{1,1}(\mathbf{R}^n)$ and $\alpha > 2 - d$ imply any $(d_\infty\text{-local})$ optimizer with compact support has Hausdorff dimension at least $2 - \alpha$. We sketch their argument briefly: the Euler-Lagrange equation satisfied by an optimizer $\mu \in \mathcal{P}(\mathbf{R}^d)$ yields $\Delta(W * \mu) \geq 0$ on $\text{spt } \mu$. Now

$$\Delta \frac{|x|^\alpha}{\alpha(\alpha - d + 2)} = |x|^{\alpha-2} + c_d(\alpha)\delta_0 \geq |x|^{\alpha-2}$$

so

$$(\alpha - d + 2) \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^{\alpha-2} d\mu(x) d\mu(y) \leq \|\Delta\phi\|_{L^\infty(\mathbf{R}^d)}.$$

But finiteness of this singular integral is known to imply any set of full μ measure has Hausdorff dimension at least $2 - \alpha$ (i.e. positive for $\alpha < 2$). Our results show the analogous conclusion fails in a nonempty range $\alpha \in [\alpha_{\Delta^d}, 2)$ on the projective sphere, reflecting its curved and compact geometry and providing some further evidence supporting the continuous *Fejes Tóth conjecture* $\alpha_{\Delta^d} = 1$.

Lastly, we note that Fejes Tóth actually considered the maximization problem over the discrete domain $\mathcal{P}_N^-(\mathbf{S}^d)$ for each $N \in \mathbf{N}$. In this setup it seems that majorization approach which Bilyk et al describe in the “Appendix A” below does not apply (unless N is a multiple of $d + 1$). In Section 4 we shall address this by giving corresponding results regarding the existence of an N -dependent threshold exponent $\alpha_{\Delta^d}(N) \in [1, \infty)$ for this problem when $N > d + 1$ with Fejes Tóth’s conjectures becoming equivalent to the assertion $\alpha_{\Delta^d}(N) = 1$; see Lemma 4.1 and Theorem 4.5.

2 Measures on an orthonormal basis are local energy maximizers

In this section we show that the conjectured maximizer of (1.5) for $\alpha = 1$ is—up to projective rotations—a strict local maximizer for all $\alpha > 1$. Moreover, the same is true for all measures which share its support. For $1 \leq p < +\infty$ define the L^p -Kantorovich–Rubinstein–Wasserstein (optimal transport) distance between $\mu, \nu \in \mathcal{P}(\mathbf{S}^d)$ by

$$d_p(\mu, \nu) := \inf_{\gamma \in \Gamma(\mu, \nu)} \left(\int_{\mathbf{S}^d \times \mathbf{S}^d} \rho(x, y)^p d\gamma(x, y) \right)^{1/p}, \quad (2.1)$$

where the infimum is taken over the set $\Gamma(\mu, \nu)$ of joint probability measures on $\mathbf{S}^d \times \mathbf{S}^d$ having μ and ν as their left and right marginals. For $p \neq \infty$, the distance d_p is well-known to metrize narrow convergence (against continuous bounded test functions, e.g. Theorem 7.12 of [23]), so $\mathcal{P}(\mathbf{S}^d)$ becomes a compact metric space under d_p . The limit

$$d_\infty(\mu, \nu) := \inf_{\gamma \in \Gamma(\mu, \nu)} \sup_{(x, y) \in \text{spt } \gamma} \rho(x, y) \quad (2.2)$$

is also a distance, but metrizes a much finer and non-compact topology on $\mathcal{P}(\mathbf{S}^d)$ (but not on $\mathcal{P}_N^-(\mathbf{S}^d)$, as we shall see in Lemma 4.4). For $\alpha > 1$, this finer topology allows us to establish local energy maximality of even the wildly unbalanced measures in $\mathcal{P}_\Delta(\mathbf{S}^d)$, echoing its uses in other settings [3, 17, 20].

Let $e_0 = (0, 0, \dots, 0, 1)$, $e_1 = (1, 0, \dots, 0)$, \dots , $e_d = (0, \dots, 0, 1, 0)$ be the standard basis of \mathbf{R}^{d+1} . Let $D(x, r)$ and $B(x, r)$ denote the open balls of center x and radius r in \mathbf{S}^d and \mathbf{R}^d respectively, and denote the Euclidean norm by $|\cdot|$. The following lemma is standard:

Lemma 2.1 (Barycenter characterization) *Let μ be a Borel probability measure on \mathbf{R} and $c \in L^1(\mathbf{R}, d\mu)$. Then*

$$\int |x - c(y)| d\mu(y) \geq \left| x - \int c(y) d\mu(y) \right| \text{ for all } x \in \mathbf{R}. \quad (2.3)$$

Proof Jensen's inequality. \square

The function $x \in \mathbf{S}^d \mapsto \Lambda(x, e_1)$ peaks like a roof at the equator $e_1^\perp \cap \mathbf{S}^d$, where $x^\perp := \{y \in \mathbf{R}^{d+1} \mid x \cdot y = 0\}$. Thus, near $e_0 \in \mathbf{S}^d$, the potential corresponding to unit Dirac masses at each of the other basis vectors e_i behaves asymptotically like the ℓ^1 norm on the tangent space $T_{e_0}\mathbf{S}^d$, which obviously dominates the ℓ^2 (Riemannian) norm there. Thus $C' < 1$ yields

$$\frac{\pi}{2} \sum_{i=1}^d (1 - \Lambda(x, e_i)) \sim \sum_{i=1}^d |x \cdot e_i| \geq C' \left(\sum_{i=1}^d |x \cdot e_i|^2 \right)^{1/2}, \quad (2.4)$$

with the final inequality being strict unless both sides vanish, in which case x is a multiple of e_0 . The next lemma gives a perturbation of this result that plays a crucial role in our local stability argument.

Proposition 2.2 (Recentred potentials near conjectured optimizer) *Given $0 < C < \frac{2}{\pi}$, there exists $r(d, C) > 0$ such that: if $v_i \in \mathcal{P}(D(e_i, r))$ for $r < r(d, C)$ and each $i = 1, \dots, d$, (i.e. v_i is a probability measure on \mathbf{S}^d with $v_i(D(e_i, r)) = 1$), then there exists $\bar{x} = \bar{x}(v_1, \dots, v_d) \in \mathbf{S}^d$ satisfying*

$$\sum_{i=1}^d \int (1 - \Lambda(x, y)) dv_i(y) \geq C \rho(x, \bar{x}) \quad \forall x \in D(e_0, r). \quad (2.5)$$

Finally, $\bar{x} \rightarrow e_0$ as $r \rightarrow 0$.

Proof Fix the Riemannian exponential map

$$\exp_{e_0} v = e_0 \cos |v| + \frac{v}{|v|} \sin |v| \quad (2.6)$$

from the tangent space $T_{e_0}M = e_0^\perp \cong \mathbf{R}^d \subset \mathbf{R}^{d+1}$ onto \mathbf{S}^d . Let $i \in \{1, \dots, d\}$ and r be small. For each $y \in D(e_i, r)$ and small $v \in e_0^\perp$, consider the function

$V_y(v) := 1 - \Lambda(\exp_{e_0} v, y)$ and its zero set $Z_y \subset e_0^\perp$. Note $\exp_{e_0} Z_y = y^\perp \cap \mathbf{S}^d = \{x \mid \Lambda(x, y) = 1\} = \{x \mid \rho(x, y) = \frac{\pi}{2}\}$.

Let Q be the hypercube $[-s, s]^d \subset e_0^\perp$ for $s > 0$. For $r \ll s \ll 1$ both sufficiently small, $Z_y \cap Q$ can be viewed as the graph of a smooth function $\zeta_y : [-s, s]^{d-1} \rightarrow [-s, s]$, that is, $v = (v_1, \dots, v_d) \in Z_y$ if and only if $v_i = \zeta_y(v_{-i})$ where $v_{-i} := (v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_d)$. Here the ζ_y are uniformly smooth, hence $\zeta_y \rightarrow 0 = \zeta_{e_i}$ in smooth norms as $r \rightarrow 0$, our notation $r \ll s$ signifying that r tends to zero faster than s . Since the linearization of (2.6) at $v = 0$ gives the identity map, from the definition of Λ and $C < \frac{2}{\pi}$, observe if r, s are sufficiently small

$$V_y(v) \geq C|f_y(v)| \quad \text{for all } v \in Q$$

where $f_y(v) := v_i - \zeta_y(v_{-i})$ on $v = (v_1, \dots, v_d) \in Q$. This implies

$$F_i(v) := \int V_y(v) dv_i(y) \geq C \int |f_y(v)| dv_i(y) \quad \text{for all } v \in Q.$$

Let $\xi_i : [-s, s]^{d-1} \rightarrow [-s, s]$ be defined by $\xi_i(v_{-i}) = \int \zeta_y(v_{-i}) dv_i(y)$, and $Z^i \subset Q$ be its graph $Z^i := \{(v_1, \dots, v_d) \in Q \mid v_i = \xi_i(v_{-i})\}$. Define a function g_i on Q by $g_i(v_1, \dots, v_d) = v_i - \xi_i(v_{-i})$. Then by Lemma 2.1, we find

$$\int |f_y| dv_i(y) \geq |g_i| \quad \text{on } Q.$$

From uniformity in i of smoothness of ξ_i , it follows that $|\xi_i|$ and $|\nabla \xi_i|$ converge uniformly to zero as $r \rightarrow 0$ (regardless of the choice of v_i), and their graphs are orthogonal in the limit. Thus $v^r := \bigcap_{i=1}^d Z^i$ is a singleton for small enough r and $v^r \rightarrow 0$ as $r \rightarrow 0$.

Composing the map $v \in e_0^\perp \mapsto G^r(v) = (g_1(v), \dots, g_d(v))$ with $\exp_{e_0}^{-1}$ gives a $(v_i)_{i=1}^d$ -dependent coordinate chart taking $\bar{x} := \exp_{e_0} v^r$ to $0 \in \mathbf{R}^d$ and converging in smooth norms as $r \rightarrow 0$ to the Riemannian normal coordinates $G^0(v) = (v_1, \dots, v_d)$ at e_0 . Taylor expansion yields

$$G^r(v) = DG^r(v^r)(v - v^r) + O(|v - v^r|^2)$$

where $DG^r(v^r) = I + o(1)$ as $r \rightarrow 0$. Noting inequality (2.4), given $C' \in (0, 1)$, taking $r \ll s \ll 1$ small enough therefore yields

$$\begin{aligned} \sum_{i=1}^d |g_i(v)| &\geq \left(\sum_{i=1}^d g_i(v)^2 \right)^{1/2} \\ &\geq \frac{C' + 1}{2} |v - v^r| \\ &\geq C' \rho(\bar{x}, \exp_{e_0} v) \quad \text{for all } v \in Q. \end{aligned}$$

Combining the foregoing, we obtain

$$\sum_{i=1}^d F_i(v) \geq C \sum_{i=1}^d |g_i(v)| \geq CC' \rho(\bar{x}, \exp_{e_0} v) \text{ for all } v \in Q$$

which translates to (2.5) on \mathbf{S}^d via the exponential map (2.6).

Remark 2.3 (Conditions for equality) Varying $0 < C < \frac{2}{\pi}$ makes it clear that (2.5) is saturated only when both sides vanish.

Recall that $\mathcal{P}_\Delta(\mathbf{S}^d)$ consists of probability measures $\hat{\mu}$ whose support covers an orthonormal basis $V \subset \mathbf{R}^{d+1}$ and is contained in the double $V \cup -V$ of that basis. For $\alpha > 1$, the following theorem provides a d_∞ -ball around each such $\hat{\mu}$ on which it maximizes the energy $E_\alpha(\mu)$ essentially uniquely (i.e. uniquely among probability measures on the projective sphere, apart from rotations). It is inspired by Corollary 4.3 of [17], which gives the analogous result in a different context.

Theorem 2.4 (d_∞ -local energy maximizers) *Given $1 < \alpha < \infty$, $m > 0$ and $d \in \mathbf{N}$, there exists $r = r(d, \alpha, m) > 0$ such that for every $\beta \geq \alpha$ and $\xi, \hat{\xi} \in \mathcal{P}(\mathbf{S}^d)$ with $d_\infty(\xi, \hat{\xi}) < r$: if $\hat{\xi} \in \mathcal{P}_\Delta(\mathbf{S}^d)$ and $\hat{\xi}(\{z, -z\}) \geq m$ for each $z \in \text{spt } \hat{\xi}$, then $E_\beta(\xi) \leq E_\beta(\hat{\xi})$ and the inequality is strict unless ξ is a rotation of $\hat{\xi}$.*

Proof Observe it is sufficient to prove for $\beta = \alpha$ since $E_\beta(\xi) \leq E_\alpha(\xi)$ for all $\beta \geq \alpha$ and $\xi \in \mathcal{P}(\mathbf{S}^d)$, while $E_\beta(\hat{\xi}) = E_\alpha(\hat{\xi})$. Thus we set $\beta = \alpha$. Fix $\hat{\xi} \in \mathcal{P}_\Delta(\mathbf{S}^d)$ and assume $\xi \in \mathcal{P}(\mathbf{S}^d)$ satisfies $d_\infty(\hat{\xi}, \xi) < r$ for some $0 < r \ll \pi/4$ to be specified later. Again the abbreviation $r \ll \pi/4$ means “for r sufficiently small.”

By rotation, we may assume $\hat{\xi} = \sum_{i=0}^d (p_i \delta_{e_i} + q_i \delta_{-e_i})$. By transferring the mass at $-e_i$ to e_i , define $\hat{\mu} = \sum_{i=0}^d m_i \delta_{e_i}$ with $m_i = p_i + q_i > 0$, and set $m := \min_i m_i$. We similarly transform ξ to μ , retaining $d_\infty(\mu, \hat{\mu}) < r$ with $E_\alpha(\hat{\xi}) = E_\alpha(\hat{\mu})$ and $E_\alpha(\xi) = E_\alpha(\mu)$. (We can alternately consider that we convert $\hat{\xi}$ and ξ to measures $\hat{\omega}$ and ω on the projective space \mathbf{RP}^d , by pushing them forward through the map $z \in \mathbf{S}^d \rightarrow \tilde{z} = \{z, -z\} \in \mathbf{RP}^d$. This neither increases their separation nor changes their energy, when the obvious definitions of d_∞ and E_α are adopted for measures on projective space. We shall derive conditions under which ω must be a rotation of $\hat{\omega}$, hence supported at $d + 1$ well-separated points. When $d_\infty(\xi, \hat{\xi}) < \pi/4$ this in turn implies ξ is a rotation of $\hat{\xi}$.)

We need to show that, for r sufficiently small, $d_\infty(\hat{\mu}, \mu) < r$ implies $E_\alpha(\hat{\mu}) \geq E_\alpha(\mu)$ and the inequality is strict unless μ is a rotation of $\hat{\mu}$, meaning in particular $\mu \in \mathcal{P}_{\text{on}}(\mathbf{S}^d)$ as well. Note that, since $d_\infty(\mu, \hat{\mu}) < r \ll \pi/4$, we have $\mu(D(e_i, r)) = m_i$ for all i . Let $\mu_i = \mu|_{D(e_i, r)}$ be the restriction and $v_i = m_i^{-1} \mu_i$ its normalization. Setting $F(\mu) = 2(E_\alpha(\mu) - E_\alpha(\hat{\mu}))$ and $\Lambda^\alpha * \mu_j(x) := \int \Lambda^\alpha(x, y) d\mu_j(y)$, observe

$$F(\mu) = \sum_{j=0}^d \left[\int (\Lambda^\alpha * \mu_j) d\mu_j + \sum_{i \neq j} \iint (\Lambda^\alpha(x_i, x_j) - 1) d\mu_i(x_i) d\mu_j(x_j) \right].$$

By Proposition 2.2, for any $C \in (0, \frac{2}{\pi})$ we have, recalling $m := \min_i m_i$,

$$\begin{aligned} & \sum_{j=0}^d \sum_{i \neq j} \iint (\Lambda^\alpha(x_i, x_j) - 1) d\mu_i(x_i) d\mu_j(x_j) \\ &= \sum_{j=0}^d \sum_{i \neq j} m_i m_j \iint (\Lambda^\alpha(x_i, x_j) - 1) dv_i(x_i) dv_j(x_j) \\ &\leq -Cm^2 \sum_{j=0}^d \int \rho(\bar{x}_j, x_j) dv_j(x_j) \end{aligned}$$

for some $\{\bar{x}_j\}_{j=0}^d \subset \mathbf{S}^d$, if r is sufficiently small.

Next, let us address the localized self-interaction terms $\int (\Lambda^\alpha * \mu_j) d\mu_j$. For $x, x' \in D(e_j, r)$,

$$\begin{aligned} & \iint \Lambda^\alpha(x, x') d\mu_j(x) d\mu_j(x') \\ &= \left(\frac{2}{\pi}\right)^\alpha m_j^2 \iint \rho(x, x')^\alpha dv_j(x) dv_j(x') \\ &\leq C' \int \rho(x, \bar{x}_j)^\alpha dv_j(x) \end{aligned}$$

with $C' = (\frac{4}{\pi})^\alpha$, since $\alpha \geq 1$ yields $2^{1-\alpha} \rho(x, x')^\alpha \leq \rho(x, \bar{x}_j)^\alpha + \rho(\bar{x}_j, x')^\alpha$ by convexity. Then since $\alpha > 1$ and $\bar{x}_j \rightarrow e_j$ as $r \rightarrow 0$, for any $\epsilon > 0$ we have

$$\int \rho(x, \bar{x}_j)^\alpha dv_j(x) \leq \epsilon \int \rho(x, \bar{x}_j) dv_j(x)$$

if r is small enough. Combining, we obtain

$$F(\mu) \leq (C'\epsilon - Cm^2) \sum_{j=0}^d \int \rho(x, \bar{x}_j) dv_j(x).$$

By taking $\epsilon < Cm^2/C'$ we have $F(\mu) \leq 0$ as desired. Moreover $F(\mu) < 0$ unless $\int \rho(x, \bar{x}_j) dv_j(x) = 0$ for all j , in which case $v_j = \delta_{\bar{x}_j}$ for all j . Recalling its definition, $F(\mu) = 0$ then implies $\rho(\bar{x}_i, \bar{x}_j) = \pi/2$ for all $i \neq j$, that is, $F(\mu) = 0$ if and only if μ is a rotation of $\hat{\mu}$. \square

Remark 2.5 (Sharp threshold exponent for local stability) When $\alpha = 1$, the proof of Lemma 1.1 shows the conclusion of Theorem 2.4 to fail, in the sense that even when $\hat{\xi} \in \mathcal{P}_{\Delta}^-(\mathbf{S}^d)$ so that $m = \frac{1}{d+1}$, $E_1(\xi) = E_1(\hat{\xi})$ does not imply ξ is a rotation of $\hat{\xi}$, no matter how small $d_\infty(\xi, \hat{\xi})$ is.

The remaining sections of this paper establish $\alpha_{\Delta^d} < \infty$. Taking this fact for granted—at least temporarily—yields:

Corollary 2.6 (Discontinuous bifurcation unless $\alpha_{\Delta^d} = 1$) *Fix $d \in \mathbf{N}$. No curve $(\mu_\alpha)_{\alpha>0}$ of optimizers*

$$\mu_\alpha \in \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_\alpha \quad (2.7)$$

can be d_∞ -continuous at $\alpha = \alpha_{\Delta^d}$ except possibly if $\alpha_{\Delta^d} = 1$.

Proof Choose any curve $(\mu_\alpha)_{\alpha>0}$ of optimizers (2.7). Lemma 1.1 provides $\alpha_{\Delta^d} \geq 1$ such that $\mu_\alpha \in \mathcal{P}_\Delta^=(\mathbf{S}^d)$ if $\alpha > \alpha_{\Delta^d}$, but not if $\alpha < \alpha_{\Delta^d}$. Theorem 2.4 provides a d_∞ -neighbourhood (in fact, tubular of radius $r = r(d, \frac{1+\alpha_{\Delta^d}}{2}, \frac{1}{m+1}) > 0$) around $\mathcal{P}_\Delta^=(\mathbf{S}^d)$ on which $\mathcal{P}_\Delta^=(\mathbf{S}^d)$ uniquely maximizes E_α for all $\alpha > \frac{1}{2}(1 + \alpha_{\Delta^d})$. Its optimality (2.7) ensures μ_α lies outside this neighbourhood whenever $\alpha < \alpha_{\Delta^d}$. Unless $(\frac{1+\alpha_{\Delta^d}}{2}, \alpha_{\Delta^d})$ is empty, this implies

$$\liminf_{\epsilon \searrow 0} d_\infty(\mu_{\alpha+\epsilon}, \mu_{\alpha-\epsilon}) \geq r > 0.$$

Thus d_∞ -continuity of $(\mu_\alpha)_{\alpha>0}$ at $\alpha = \alpha_{\Delta^d}$ implies $\alpha_{\Delta^d} \in \{1, \infty\}$. But $\alpha_{\Delta^d} = \infty$ is ruled out below (see Remark 3.7).

3 Nonunique energy maximizers at threshold exponent

In this section we show that the interval of exponents $\alpha < \infty$ for which the energy (1.5) is essentially uniquely maximized by the conjectured optimizer does not include its endpoint. We shall employ DeGiorgi's notion of Γ -convergence [12]. Since the sign conventions in this theory are normally set up so that Γ -convergence guarantees accumulation points of minimizers are minimizers, we must show $-E_\beta = \Gamma\text{-}\lim_{\alpha \rightarrow \beta} (-E_\alpha)$.

Definition 3.1 (Γ -convergence) A sequence $F_i : M \rightarrow \overline{\mathbf{R}}$ on a metric space (M, d) is said to Γ -converge to $F_\infty : M \rightarrow \overline{\mathbf{R}}$, denoted $F_\infty = \Gamma\text{-}\lim_{i \rightarrow \infty} F_i$, if (a)

$$F_\infty(\mu) \leq \liminf_{i \rightarrow \infty} F_i(\mu_i) \quad \text{whenever} \quad d(\mu_i, \mu) \rightarrow 0, \quad (3.1)$$

and (b) each $\mu \in M$ is the limit of a sequence $(\mu_i)_i \subset M$ along which

$$F_\infty(\mu) \geq \limsup_{i \rightarrow \infty} F_i(\mu_i). \quad (3.2)$$

Lemma 3.2 (Γ -convergence of energies) *The functionals $(-E_\alpha)$ Γ -converge to $(-E_\beta)$ on $(\mathcal{P}(\mathbf{S}^d), d_2)$ as $\alpha \rightarrow \beta \in [1, \infty]$. Here d_2 is from (2.1).*

Proof Let $\{\alpha_n\}_n$ be a sequence with $\lim_{n \rightarrow \infty} \alpha_n = \beta$. To show the Γ -convergence, we need to show:

$$E_\beta(\mu) \geq \limsup_{n \rightarrow \infty} E_{\alpha_n}(\mu_n) \quad \text{whenever} \quad d_2(\mu_n, \mu) \rightarrow 0, \quad (3.3)$$

and each $\mu \in \mathcal{P}(\mathbf{S}^d)$ is the limit of a sequence $(\mu_n)_n \subset \mathcal{P}(\mathbf{S}^d)$ with

$$E_\beta(\mu) \leq \liminf_{n \rightarrow \infty} E_{\alpha_n}(\mu_n). \quad (3.4)$$

If $1 \leq \beta < \infty$ more is true: in this case E_{α_n} and $-E_{\alpha_n}$ converge to E_β and $-E_\beta$ respectively since whenever $d_2(\mu_n, \mu) \rightarrow 0$ then

$$\begin{aligned} E_{\alpha_n}(\mu_n) &= \int [\Lambda^{\alpha_n} - \Lambda^\beta] d(\mu_n \otimes \mu_n) + \int \Lambda^\beta d(\mu_n \otimes \mu_n) \\ &\rightarrow \int \Lambda^\beta d(\mu \otimes \mu) =: E_\beta(\mu) \end{aligned}$$

as $n \rightarrow \infty$, noting $\|\Lambda^{\alpha_n} - \Lambda^\beta\|_\infty \rightarrow 0$ and continuity of Λ^β .

By contrast, when $\beta = \infty$, (3.4) follows from $E_\infty \leq E_{\alpha_n}$ by taking $\mu_n := \mu$ for all n . Similarly, the monotone decreasing dependence of the kernel Λ^α on α implies $\limsup_{n \rightarrow \infty} E_{\alpha_n}(\mu_n) \leq \limsup_n E_{\alpha_m}(\mu_n) = E_{\alpha_m}(\mu)$ for any $m \in \mathbf{N}$. Now $m \rightarrow \infty$ yields (3.3) by Lebesgue dominated convergence theorem. \square

Remark 3.3 (Limits of maximizers maximize limit) It is well-known [12] (and easy to see) that Lemma 3.2 implies that if $\alpha \rightarrow \beta$, any d_2 -accumulation point of $\mu_\alpha \in \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_\alpha$ must maximize E_β on $\mathcal{P}(\mathbf{S}^d)$.

Lemma 3.4 (Localizing mass of maximizers for approximating problems near that of the limit) Suppose μ_α attains the maximum (1.5) and $d_2(\mu_\alpha, \hat{\mu}) \rightarrow 0$ as $\alpha \rightarrow \beta \in (1, \infty)$. If $\hat{\mu} \in \mathcal{P}_\Delta^-(\mathbf{S}^d)$ and $r > 0$, then $\operatorname{spt}(\mu_\alpha) \subset \bigcup_{x \in \operatorname{spt} \hat{\mu}} (D(x, r) \cup D(-x, r))$ for all α sufficiently near β .

Proof Let $\{v_i\}_{i=0}^d$ be the orthonormal basis of \mathbf{R}^{d+1} such that $\operatorname{spt}(\hat{\mu}) \subset \bigcup_{i=0}^d \{v_i, -v_i\}$. We first claim the potential function $(\Lambda^\beta * \hat{\mu})(x) = \int \Lambda^\beta(x, y) d\mu(y)$ attains its maximum precisely on the set $\bigcup_{i=0}^d \{v_i, -v_i\}$. Indeed, $\Lambda^\beta * \hat{\mu}$ is an equally weighted sum of $d + 1$ potentials $\Lambda^\beta * \delta_{v_i}$, each of which is smooth and has a (non-vanishing) non-negative definite Hessian away from $(\pm v_i$ and) the equatorial great sphere $v_i^\perp \cap \mathbf{S}^d$ —which coincides with the cut locus of v_i on \mathbf{PR}^d . Thus the only local maxima of $\Lambda^\beta * \hat{\mu}$ on \mathbf{S}^d must lie on $\bigcup_{i=0}^d v_i^\perp$. However $\Lambda^\beta * \delta_{v_0}$ attains its maximum value of 1 throughout the great sphere $\mathbf{S}^d \cap v_0^\perp$, and it is easy to see by induction on dimension that the local maxima of $\sum_{i=1}^d \Lambda^\beta * \delta_{v_i}$ on $\mathbf{S}^d \cap v_0^\perp$ occur precisely at v_1, \dots, v_d , to establish the claim.

Since the kernels Λ^α are equiLipschitz for α near β , as $\alpha \rightarrow \beta$, the potential functions $\Lambda^\alpha * \mu_\alpha$ converge uniformly to $\Lambda^\beta * \hat{\mu}$ on \mathbf{S}^d . Given $r > 0$, this implies that the maximum of $\Lambda^\alpha * \mu_\alpha$ occurs only in $\bigcup_{i=0}^d (D(v_i, r) \cup D(-v_i, r))$ for all α

sufficiently near β . Then the Euler-Lagrange equation due to the fact $\mu_\alpha \in \operatorname{argmax} E_\alpha$ asserts

$$\operatorname{spt}(\mu_\alpha) \subset \operatorname{argmax} \Lambda^\alpha * \mu_\alpha,$$

yielding the lemma. \square

Remark 3.5 (The mildest repulsion limit) Although we expect Lemma 3.4 to remain true when $\beta = \infty$, our proof does not extend to that case since the kernels Λ^α fail to be equiLipschitz and the continuous potentials $\Lambda^\alpha * \mu_\alpha$ cannot converge uniformly to the discontinuous limit $\Lambda^\infty * \hat{\mu}$ as $\alpha \rightarrow \infty$. Notice however, that if Lemma 3.4 holds for $\beta = \infty$, then the next proof shows Theorem 3.6 also extends to $\alpha_{\Delta^d} = \infty$. Such an extension will be relevant in Sect. 4.

Theorem 3.6 (Maximizers are not unique at threshold exponent) *If $\alpha_{\Delta^d} < \infty$, then $\mathcal{P}_\Delta^=(\mathbf{S}^d) \subset \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha_{\Delta^d}}$, and the inclusion is strict.*

Proof For $\alpha_{\Delta^d} < \infty$, the desired inclusion (1.8) follows from the definition of $\alpha_{\Delta^d} \geq 1$ in Lemma 1.1 using Remark 3.3. Our goal is therefore to show this inclusion is strict. To derive a contradiction, suppose $\mathcal{P}_\Delta^=(\mathbf{S}^d) = \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha_{\Delta^d}}$. The compactness of $\mathcal{P}(\mathbf{S}^d)$ and continuity of E_α (for the metric d_2), provide $\mu_\alpha \in \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_\alpha$ for each $\alpha \in (0, \infty)$. The same compactness provides an increasing sequence $\alpha_n \nearrow \alpha_{\Delta^d}$ and corresponding maximizers $\mu_{\alpha_n} \in \operatorname{argmax} E_{\alpha_n}$ which d_2 -converge to some $\hat{\mu} \in \operatorname{argmax} E_{\alpha_{\Delta^d}}$. By assumption $\hat{\mu} \in \mathcal{P}_\Delta^=(\mathbf{S}^d)$. Then the Localization Lemma 3.4 and Local Stability Theorem 2.4 combine to yield that for large enough n , there exists $\nu_{\alpha_n} \in \mathcal{P}_\Delta(\mathbf{S}^d)$ obtained by collapsing each bit of the mass of μ_{α_n} onto the nearest point in the support of $\hat{\mu}$ such that $\operatorname{spt}(\nu_{\alpha_n}) = \operatorname{spt}(\hat{\mu})$, $d_\infty(\mu_{\alpha_n}, \nu_{\alpha_n})$ is small and $E_{\alpha_n}(\mu_{\alpha_n}) \leq E_{\alpha_n}(\nu_{\alpha_n})$, with the inequality being strict unless $\mu_{\alpha_n} \equiv \nu_{\alpha_n}$. Moreover, since $\operatorname{spt}(\nu_{\alpha_n}) = \operatorname{spt}(\hat{\mu})$, it is well-known that $E_{\alpha_n}(\nu_{\alpha_n}) \leq E_{\alpha_n}(\hat{\mu})$ and the inequality is strict unless $\nu_{\alpha_n} \equiv \hat{\mu}$, i.e. $\nu_{\alpha_n} \in \mathcal{P}_\Delta^=(\mathbf{S}^d)$, by e.g. Perron-Frobenius (1.7). Since $\mu_{\alpha_n} \in \operatorname{argmax} E_{\alpha_n}$, the inequalities must be equalities, hence $\mathcal{P}_\Delta^=(\mathbf{S}^d) \subset \operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha_n}$ for all large n . This implies $\alpha_{\Delta^d} \leq \alpha_n$ by Lemma 1.1, contradicting the strict monotonicity $\alpha_n \nearrow \alpha_{\Delta^d}$ to establish the theorem. \square

Remark 3.7 (Finiteness of the threshold exponent) In the first version of this manuscript posted on the arXiv, we combined similar arguments with our prior results [18, 19] and a uniform cardinality bound on the support of d_2 -local maximizers for all $\alpha \geq 4$ to deduce $\alpha_{\Delta^d} < \infty$; see the next section for a similar but simpler argument in the discrete context $N < \infty$. Thus the finiteness required by Theorem 3.6 turns out not to be restrictive. In response, Bilyk et al obtained an explicit bound $\alpha_{\Delta^d} \leq 2$ using a clever majorization argument, which they were kind enough to include in the attached ‘‘Appendix A’’. Combining their work with ours yields a stronger conclusion, which might be seen as additional evidence for the continuous Fejes-Tóth conjecture $\alpha_{\Delta^d} = 1$, namely:

Corollary 3.8 (Improving Bilyk et al’s threshold exponent bound) *The threshold exponent from Lemma 1.1 satisfies $\alpha_{\Delta^d} \in [1, 2)$.*

Proof Follows from Theorems 3.6 and A.1 and Lemma 1.1. \square

Finally, we remark on the possible disconnectedness of the set of optimizers at the threshold exponent. Although the set $\mathcal{P}_{\Delta}^{\pm}(\mathbf{S}^d)$ of measures on the sphere has uncountably many d_{∞} -connected components, they are all essentially equivalent to a single measure $\hat{\mu}$. The rotates of $\hat{\mu}$ form a d_{∞} -connected set of measures on projective space $\mathbf{RP}^d = \mathbf{S}^d / \{\pm\}$. However, the results of this section and the previous one combine to show d_{∞} -connectedness of the set of energy optimizers on projective space must fail at the threshold exponent unless the continuous Fejes Tóth conjecture holds true:

Corollary 3.9 (On connectedness of the threshold set of optimizers) *Fix $d \in \mathbf{N}$. At the threshold exponent α_{Δ^d} , if the set of optimizers*

$$(\operatorname{argmax}_{\mathcal{P}(\mathbf{S}^d)} E_{\alpha_{\Delta^d}}) / \{\pm\} \quad (3.5)$$

forms a d_{∞} -connected subset of $\mathcal{P}(\mathbf{RP}^d)$, then $\alpha_{\Delta^d} = 1$.

Proof Assume $\alpha_{\Delta^d} > 1$. Theorem 2.4 then provides a d_{∞} -open neighbourhood of $\mathcal{P}_{\Delta}^{\pm}(\mathbf{S}^d)$ on which $\mathcal{P}_{\Delta}^{\pm}(\mathbf{S}^d)$ uniquely maximizes $E_{\alpha_{\Delta^d}}$. Theorem 3.6 and the finiteness of α_{Δ^d} from Remark 3.7 assert another maximizer lies outside this neighbourhood. The d_{∞} -disconnectedness of (3.5) follows, and establishes the corollary's contrapositive. \square

Of course, if the conjecture $\alpha_{\Delta^d} = 1$ holds true, we do not know whether or not the set of optimizers (3.5) is d_{∞} -connected. Indeed, the last corollary shows the continuous Fejes Tóth conjecture follows if one can establish d_{∞} -connectedness of (3.5).

4 Maximizing energy among finitely many lines (charges)

Fejes Tóth's original paper [14] considered the optimization problem $\max E_1$ not on $\mathcal{P}(\mathbf{S}^d)$, but instead over the domain of uniform discrete probabilities $\mathcal{P}_N^{\pm}(\mathbf{S}^d)$ for each $N \in \mathbf{N}$. It conjectured

$$\mathcal{P}_{N,\Delta}^{\pm}(\mathbf{S}^d) := \{\mu \mid \text{there is an orthonormal basis } \{v_i\}_{i=1}^{d+1} \text{ of } \mathbf{R}^{d+1} \text{ and } \{x_i\}_{i=1}^N \text{ such that } \mu = \frac{1}{N} \sum_{i=1}^N \delta_{x_i} \text{ and } x_i \in \{v_j, -v_j\} \text{ if } i \equiv j \pmod{d+1}\}$$

maximizes E_1 over $\mathcal{P}_N^{\pm}(\mathbf{S}^d)$. Notice $\mu \in \mathcal{P}_{N,\Delta}^{\pm}(\mathbf{S}^d)$ iff $\mu \equiv \psi$ where ψ distributes N particles of equal mass $1/N$ on an orthonormal basis as uniformly as possible.

This problem admits an analog of Lemma 1.1, whose similar proof is omitted:

Lemma 4.1 (Threshold exponent for discrete equidistribution over maximal simplices) *Given $d, N \in \mathbf{N}$, there exists a unique $\alpha_{\Delta^d}(N) \in [0, \infty]$ such that $0 <$*

$\alpha < \alpha_{\Delta^d}(N)$ implies $\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$ disjoint from $\operatorname{argmax}_{\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)} E_\alpha$, whereas $\alpha_{\Delta^d} < \alpha$ implies

$$\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d) = \operatorname{argmax}_{\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)} E_\alpha. \quad (4.1)$$

If $N > d + 1$ then (4.1) fails for $\alpha = 1$, hence $\alpha_{\Delta^d}(N) \geq 1$.

In terms of this N -dependent threshold exponent, Fejes Tóth's conjecture reduces to the assertion that $N > d + 1$ implies $\alpha_{\Delta^d}(N) = 1$.

The majorization method of the ‘‘Appendix A’’ below does not seem to apply in this setup unless N is a multiple of $d + 1$. Thus for N indivisible by $d + 1$ it is not clear to us whether $\alpha_{\Delta^d}(N) < 2$. However, we shall adapt the strategy above to show that $\alpha_{\Delta^d}(N) < \infty$, that is for each N , (4.1) holds for all sufficiently large finite α .

To this end, we first recall our results [18, Theorem 1.4] on the mildest repulsion limit $\alpha = \infty$, which include the assertion that (4.1) holds when $\alpha = \infty$. (We subsequently learned from the authors of our ‘‘Appendix A’’ that this conclusion can alternately be obtained as a consequence of Turan's theorem, which asserts that, among graphs with N vertices and no $(d + 2)$ -cliques, the number of edges is uniquely maximized by the complete $(d + 1)$ -partite graph $K_{k_1, \dots, k_{d+1}}$ with $|k_i - k_j| \leq 1$ for all $i, j \in \{1, \dots, d + 1\}$ [1, 22].)

The proof of the following lemma is virtually verbatim to that of Lemma 3.2, if one replaces E_β with E_∞ and $\mathcal{P}(\mathbf{S}^d)$ with $\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$, so we omit it here.

Lemma 4.2 (Γ -convergence of discrete energies) *Fix $N \in \mathbf{N}$. The functionals $(-E_\alpha)$ Γ -converge to $(-E_\infty)$ on $(\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d), d_2)$ as $\alpha \rightarrow \infty$. Here d_2 is from (2.1).*

As in Remark 3.3, this implies any d_2 -accumulation point μ of $\mu_\alpha \in \operatorname{argmax}_{\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)} E_\alpha$ as $\alpha \rightarrow \infty$ belongs to $\operatorname{argmax}_{\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)} E_\infty = \mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$. But since $\mu_\alpha \in \mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$, the following lemma (which may be folklore to experts) shows $d_2(\mu_\alpha, \mu) \rightarrow 0$ yields $d_\infty(\mu_\alpha, \mu) \rightarrow 0$ as $\alpha \rightarrow \infty$.

Remark 4.3 The sphere \mathbf{S}^d plays no special role, and could be replaced by an arbitrary complete separable metric space in the next lemma.

Lemma 4.4 (d_∞ metrizes the narrow topology on $\mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$) *Given $1 \leq p < \infty$, any $\mu, \nu \in \mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$ satisfy*

$$N^{-1/p} d_\infty(\mu, \nu) \leq d_p(\mu, \nu) \leq d_\infty(\mu, \nu).$$

Proof One direction is standard: Jensen's inequality implies $d_p \leq d_q$ for all $1 \leq p < q < \infty$, hence $d_p \leq d_\infty = \lim_{q \rightarrow \infty} d_q$ even on the larger space $\mathcal{P}(\mathbf{S}^d)$. Conversely, $\mu, \nu \in \mathcal{P}_{N,\Delta}^{\overline{=}}(\mathbf{S}^d)$ satisfy $\mu = \frac{1}{N} \sum_{i=1}^N \delta_{x^i}$ and $\nu = \frac{1}{N} \sum_{j=1}^N \delta_{y^j}$, so the infimum (2.1) over $\gamma \in \Gamma(\mu, \nu)$ defining $d_p(\mu, \nu)$ reduces to a finite-dimensional linear program for a doubly stochastic $N \times N$ matrix with entries $G^{ij} = \gamma[\{(x^i, y^j)\}]$. This infimum is attained by a permutation matrix G_p , as a consequence of the Birkhoff-von Neumann characterization of extremal doubly stochastic matrices [10]. Reorder

the points $(y^j)_{j=1}^N$ so that G_p is the identity matrix. Taking the corresponding measure $\gamma_p \in \Gamma(\mu, \nu)$ as a competitor bounding the distance $d_q(\mu, \nu)$, the limit $q \rightarrow \infty$ (or (2.2) directly) yields

$$\begin{aligned} Nd_p(\mu, \nu)^p &= \sum_{i=1}^N \rho(x^i, y^i)^p \\ &\geq \max_{1 \leq i \leq N} \rho(x^i, y^i)^p \\ &\geq d_\infty(\mu, \nu)^p \end{aligned}$$

as desired. \square

Using this d_∞ -convergence in place of Lemma 3.4 and noting Remark 3.5, the same proof adapts Theorem 2.4 to this context, yielding the following conclusion:

Theorem 4.5 (Finiteness of discrete threshold exponent) *Given $d, N \in \mathbb{N}$, the threshold exponent from Lemma 4.1 is finite $\alpha_{\Delta^d}(N) \in [0, \infty)$ and the containment $\mathcal{P}_{N, \Delta}^=(\mathbf{S}^d) \subset \operatorname{argmax}_{\mathcal{P}_{\bar{N}}^=(\mathbf{S}^d)} E_{\alpha_{\Delta^d}(N)}$ is strict.*

The obvious analogs of the discontinuity / disconnectedness results of Corollaries 2.6 and 3.9 extend to this discrete (i.e. $N < \infty$) setting.

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Appendix A. By Dmitriy Bilyk, Alexey Glazyrin, Ryan Matzke, Josiah Park, and Oleksandr Vlasiuk

Theorem A.1 (Estimating the threshold exponent: $\alpha_{\Delta^d} \leq 2$) *For every $\alpha \geq 2$, the set of maximizers of (1.5) is precisely $\mathcal{P}_{\Delta}^=(\mathbf{S}^d)$.*

Proof For $t \in [-1, 1]$ set $f_\alpha(t) = (\frac{2}{\pi} \arccos |t|)^\alpha$ and $g(t) = 1 - t^2$. We claim

$$g \geq f_\alpha \text{ on } [-1, 1] \text{ and } \{g = f_\alpha\} = \{-1, 0, 1\} \iff \alpha \geq 2. \quad (\text{A.1})$$

Indeed, setting $h_\alpha(t) := g(t)^{1/\alpha} - f_\alpha(t)^{1/\alpha}$, the computation $h_2''(t) = (2t\pi^{-1} - 1)(1 - t^2)^{-3/2}$ shows $h_2(t)$ to be strictly concave on the interval $t \in [0, 1]$ and to vanish at both endpoints. For $\alpha = 2$ this establishes (A.1). For $\alpha > 2$, the same conclusion then follows from $\frac{dh_\alpha}{da}(t) \geq 0$. For $\alpha < 2$ we have $\lim_{t \nearrow 1} f'_\alpha(t) = -\infty < g'(1)$ and $f_\alpha(1) = 0 = g(1)$, thus domination of f_α by g fails, confirming the reverse implication in (A.1).

Now (1.4) may be rewritten in the form $E_\alpha(\mu) = F_{f_\alpha}(\mu)$ where

$$F_f(\mu) := \iint f(x \cdot y) d\mu(x) d\mu(y).$$

Let $\mu \in \mathcal{P}(\mathbf{S}^d)$, σ be the uniform probability on \mathbf{S}^d , and $\hat{\mu} \in \mathcal{P}_\Delta^\equiv(\mathbf{S}^d)$. For $\alpha \geq 2$ we claim

$$F_{f_\alpha}(\mu) \leq F_g(\mu) \leq F_g(\sigma) = F_g(\hat{\mu}) = F_{f_\alpha}(\hat{\mu}) \quad (\text{A.2})$$

where the middle two (in)equalities for g are known and reproved below, while the first and last follow from (A.1)—which also makes the first inequality strict unless μ lies in the narrow closure of $\mathcal{P}_\Delta(\mathbf{S}^d)$. On the other hand, for $\mu \in \overline{\mathcal{P}_\Delta(\mathbf{S}^d)}$, (1.7) implies that the second inequality in (A.2) becomes strict unless $\mu \in \mathcal{P}_\Delta^\equiv(\mathbf{S}^d)$.

It remains to establish the middle two (in)equalities in (A.2) for g , which can be done in various ways, c.f. [4]. For example, defining the symmetric $(d+1) \times (d+1)$ matrix $I(\mu)$ by

$$I^{ij}(\mu) = \int_{\mathbf{S}^d} x^i x^j d\mu(x),$$

the Cauchy–Schwartz inequality for the Hilbert–Schmidt norm yields

$$\begin{aligned} \iint (x \cdot y)^2 d\mu(x) d\mu(y) &= \text{Tr}(I(\mu)^2) \\ &\geq \frac{1}{d+1} (\text{Tr } I(\mu))^2 \\ &= \frac{1}{d+1} \end{aligned}$$

since $\text{Tr } I(\mu) = |x|^2 = 1$ on \mathbf{S}^d . If $I(\mu)$ is a multiple of the identity matrix—as for $\mu \in \{\hat{\mu}, \sigma\}$ —then equality holds. This establishes (A.2) and completes the proof. \square


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