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Optimal simplices and codes in projective spaces

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We find many *tight* codes in compact spaces, in other words, optimal codes whose optimality follows from linear programming bounds. In particular, we show the existence (and abundance) of several hitherto unknown families of simplices in quaternionic projective spaces and the octonionic projective plane. The most noteworthy cases are 15–point simplices in $\mathbb{HP}^2$ and 27–point simplices in $\mathbb{OP}^2$, both of which are the largest simplices and the smallest 2–designs possible in their respective spaces. These codes are all universally optimal, by a theorem of Cohn and Kumar. We also show the existence of several positive-dimensional families of simplices in the Grassmannians of subspaces of $\mathbb{R}^n$ with $n \le 8$; close numerical approximations to these families had been found by Conway, Hardin and Sloane, but no proof of existence was known. Our existence proofs are computer-assisted, and the main tool is a variant of the Newton–Kantorovich theorem. This effective implicit function theorem shows, in favorable conditions, that every approximate solution to a set of polynomial equations has a nearby exact solution. Finally, we also exhibit a few explicit codes, including a configuration of 39 points in $\mathbb{OP}^2$ that form a maximal system of mutually unbiased bases. This is the last tight code in $\mathbb{OP}^2$ whose existence had been previously conjectured but not resolved.

51M16, 52C17; 65G20, 49M15

1 Introduction

The study of codes in spaces such as spheres, projective spaces and Grassmannians has been the focus of much interest recently, involving an interplay of methods from many aspects of mathematics, physics and computer science; see the papers by Bachoc, Nebe, de Oliveira Filho and Vallentin [9; 8]; Bondarenko, Radchenko and Viazovska [16]; Bowick and Giomi [17]; Renes [65]; Mixon, Quinn, Kiyavash and Fickus [59] and Fouvry, Kowalski and Michel [38]. Given a compact metric space X, the basic question is how to arrange N points in X so as to maximize the minimal distance between them. A finite point configuration is called a *code*, and an *optimal code* $\mathcal{C}$ maximizes the minimal distance between its points given its size $|\mathcal{C}|$. Finding optimal codes is a

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central problem in coding theory. Even when X is finite (for example, the cube $\{0,1\}^n$ under Hamming distance), this optimization problem is generally intractable, and it is even more difficult when X is infinite.

Most of the known optimality theorems have been proved using linear programming bounds, and we are especially interested in codes for which these bounds are sharp. We call them *tight* codes.[1] The class of tight codes includes many of the most remarkable codes known, such as the icosahedron and the E_8 root system.

In this paper, we explore the landscape of tight codes in projective spaces. We devote most of our attention to regular simplices (that is, collections of equidistant points). Tight simplices correspond to tight equiangular frames (see Sustik, Tropp, Dhillon and Heath [70]), which have applications in signal processing and sparse approximation, and they also capture interesting invariants of their ambient spaces. Furthermore, they seem to be by far the most widespread sort of tight codes.

In real and complex projective spaces, tight simplices occur only sporadically. All known constructions are based on geometric, group-theoretic or combinatorial properties that depend delicately on the number of points and the dimension of the projective space. By contrast, we find a surprising new phenomenon in quaternionic and octonionic spaces: in each dimension, there are substantial intervals of sizes for which tight simplices always seem to exist. For instance, in $\mathbb{HP}^2$ we show that tight simplices exist for N points with $1 \le N \le 13$ or $N = 15$, while in $\mathbb{HP}^3$ we show existence for $1 \le N \le 21$.

This behavior cannot plausibly be explained using the sorts of constructions that work in real and complex spaces. In fact, the new tight simplices exhibit little structure and seem to exist not for any special reason, but rather because of parameter counting: they can be characterized by systems of equations with more variables than constraints. Making this heuristic precise, and indeed extracting any proof from this approach, requires a delicate choice of constraints. Much of our paper is devoted to identifying and analyzing such a choice. We do not know how to prove that these new simplices exist in all dimensions, but we prove existence in many hitherto unknown cases. We also extend our methods to handle some exceptional cases that are particularly subtle.

Our results settle several open problems dating back to the early 1980s, while raising new questions.

[1] The word "tight" is used for a related but more restrictive concept in the theory of designs. We use the same word here for lack of a good substitute. This makes "tight" a noncompositional adjective, much like "optimal": codes and designs are both just sets of points, so every code is a design and vice versa, but a tight code is not necessarily a tight design. (However, one can show that every tight design is a tight code.)

(a) We show the existence of a 15–point simplex in $\mathbb{HP}^2$ (Theorem 4.12) and a 27–point simplex in $\mathbb{OP}^2$ (Theorem 5.9). These simplices are not only optimal codes, but also the largest possible simplices in their ambient spaces. For comparison, the six diagonals of an icosahedron form the largest simplex in $\mathbb{RP}^2$, and the largest simplex in $\mathbb{CP}^2$ has size nine. The real and complex simplices have long been known, but the quaternionic and octonionic simplices had been conjectured not to exist by Hoggar [43, page 251].

(b) These two codes are also tight 2–designs, which makes them analogues of "symmetric, informationally complete, positive operator-valued measures" (SIC-POVMs). SIC-POVMs are d^2–point simplices in $\mathbb{CP}^{d-1}$, which play an important role in quantum information theory (see Renes, Blume-Kohout, Scott and Caves [67]). Zauner has conjectured that SIC-POVMs exist for each d (a problem analogous in some ways to the existence of Hadamard matrices), but his conjecture remains tantalizingly out of reach; see Appleby, Fuchs and Zhu [4]. Examples of SIC-POVMs have been algebraically constructed in low dimensions (up to $d = 16$ and a few larger cases) and numerically approximated for $d \leq 67$, but no infinite families are known; see Scott and Grassl [69] and Appleby, Bengtsson, Brierley, Ericsson, Grassl and Larsson [3]. Our results do not apply directly to Zauner's conjecture, but rather they suggest that the analogous question in quaternionic projective spaces has an entirely different character: tight 2–designs in $\mathbb{HP}^{d-1}$ do not seem to exist for $d > 3$.

(c) An intriguing phenomenon we have observed is the apparent nonexistence of 14–point tight simplices in $\mathbb{HP}^2$ (Conjecture 4.13) and 26–point tight simplices in $\mathbb{OP}^2$ (Conjecture 5.10), when all other sizes up to the maximum (15 or 27, respectively) occur. We have no explanation for why the second largest possible size should not occur. We observe the same phenomenon for the Grassmannian $G(2,4)$, which bolsters our confidence that it is a genuine pattern.

(d) More generally, we prove the existence of many tight simplices in real Grassmannians (Theorems 6.4 and 6.6–6.8). Such simplices were conjectured to exist by Conway, Hardin and Sloane [31] based on numerical evidence, and we show how parameter counting explains this phenomenon. As in projective spaces, the difficulty lies in finding the right constraints, so that the problem becomes amenable to rigorous proof.

(e) Finally, we give a few explicit constructions of other codes, including a construction for a set of 13 mutually unbiased bases in $\mathbb{OP}^2$ (Theorem 8.3). They had been conjectured to exist (see Hoggar [44, page 35]), but no construction was previously known.

In contrast to the usual algebraic methods for constructing tight codes, we take a rather different approach to show the existence of families of simplices. We use a general *effective* implicit function theorem (that is, one with explicit bounds), which allows us to show the existence of a real solution to a system of polynomial equations near an approximate solution. Furthermore, it proves that the space of solutions is a smooth manifold near the approximate solution and tells us its dimension. Using this approach, we prove the existence of tight simplices by computing numerical approximations and then applying the existence theorem.[2]

The idea of making the implicit function theorem effective goes back to the Newton–Kantorovich theorem (see Kantorovich [49]), but applying it in this geometric setting allows us to establish many new results, for which algebraic constructions seem out of reach. The closest predecessor to our applications that we are aware of is a sequence of papers by Chen and Womersley [25]; Chen [23]; An, Chen, Sloan and Womersley [1] and Chen, Frommer and Lang [24], on the existence of spherical t–designs on S^2 with at least $(t+1)^2$ points. These papers also use a Newton–Kantorovich variant, applied in a case in which there are approximately twice as many variables as constraints: the space of N–point configurations on S^2 has dimension $2N-3$ for $N \geq 3$, and the t–design condition imposes $(t+1)^2-1$ constraints (since that is the dimension of the space spanned by the spherical harmonics of degree 1 through t).

In Section 2 we describe linear programming bounds and recall what is known about tight codes in projective spaces over $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ and $\mathbb{O}$. An effective existence theorem, our main tool in this paper, is the subject of Section 3. Our results concerning existence of new families of projective simplices, proved using the existence theorem, are described in Sections 4 and 5. In Section 6 we use our methods to produce positive-dimensional families of simplices in real Grassmannians. We then give a discussion of the algorithms and computer programs used for these computer-assisted proofs in Section 7. Finally, we conclude in Section 8 with three explicit constructions of universally optimal codes, the most notable of which is a maximal system of mutually unbiased bases in $\mathbb{OP}^2$.

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[2]In real projective spaces, the problem is much easier: one can easily convert an approximation to an exact construction by rounding the Gram matrix. However, that fails in other projective spaces and Grassmannians. See the discussion before Proposition 2.4.

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2 Codes in projective spaces and linear programming bounds

2.1 Projective spaces over $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ and $\mathbb{O}$

If $K = \mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$, we denote by $K\mathbb{P}^{d-1} := (K^d \setminus \{0\})/K^\times$ the set of lines in K^d. That is, we identify x and $x\alpha$ for $x \in K^d \setminus \{0\}$ and $\alpha \in K^\times$. Note the convention that $K^\times$ acts on the right; this is important for the noncommutative algebra $\mathbb{H}$.

We equip K^d with the Hermitian inner product $\langle x_1, x_2\rangle = x_1^\dagger x_2$, where $\dagger$ denotes the conjugate transpose. We may represent an element of the projective space $K\mathbb{P}^{d-1}$ by a unit-length vector $x \in K^d$, and we often abuse notation by treating the element itself as such a vector. Under this identification, the *chordal distance* between two points of $K\mathbb{P}^{d-1}$ is

$$\rho(x_1, x_2) = \sqrt{1 - |\langle x_1, x_2\rangle|^2}.$$

It is not difficult to check that this formula defines a metric equivalent to the Fubini–Study metric. Specifically, if $\vartheta(x_1, x_2)$ is the geodesic distance on $K\mathbb{P}^{d-1}$ under the Fubini–Study metric, normalized so that the greatest distance between two points is π, then

$$\cos\vartheta(x_1, x_2) = 2|\langle x_1, x_2\rangle|^2 - 1$$

and

$$\rho(x_1, x_2) = \sin\left(\frac{\vartheta(x_1, x_2)}{2}\right).$$

Alternatively, elements $x \in K\mathbb{P}^{d-1}$ correspond to projection matrices $\Pi = xx^\dagger$, which are Hermitian matrices with $\Pi^2 = \Pi$ and $\operatorname{Tr}\Pi = 1$. The space $\mathcal{H}(K^d)$ of Hermitian matrices is a real vector space endowed with a positive-definite inner product

$$\langle A, B\rangle = \operatorname{Tr}\tfrac{1}{2}(AB + BA) = \operatorname{Re}\operatorname{Tr} AB.$$

Since $\operatorname{Re} ab = \operatorname{Re} ba$ for $a, b \in K$, it follows that $\operatorname{Re}\operatorname{Tr}(ABC) = \operatorname{Re}\operatorname{Tr}(CAB)$ for $A, B, C \in K^{d\times d}$; in other words, the functional $\operatorname{Re}\operatorname{Tr}$ is *cyclic invariant*. Hence, for any $x_1, x_2 \in K\mathbb{P}^{d-1}$ with associated projection matrices $\Pi_1, \Pi_2 \in \mathcal{H}(K^d)$, we have

$$\begin{aligned}\langle \Pi_1, \Pi_2 \rangle &= \operatorname{Re}\operatorname{Tr} x_1 x_1^\dagger x_2 x_2^\dagger \\ &= \operatorname{Re}\operatorname{Tr} x_2^\dagger x_1 x_1^\dagger x_2 \\ &= \operatorname{Re} \langle x_2, x_1 \rangle \langle x_1, x_2 \rangle \\ &= |\langle x_1, x_2 \rangle|^2.\end{aligned} \tag{2-1}$$

Thus the metric on $K\mathbb{P}^{d-1}$ can also be defined by $\rho(x_1, x_2) = \sqrt{1 - \langle \Pi_1, \Pi_2 \rangle}$. Equivalently, it equals $\|\Pi_1 - \Pi_2\|_F / \sqrt{2}$, where $\|\cdot\|_F$ denotes the Frobenius norm: $\|A\|_F = \left(\sum_{i,j} |A_{ij}|^2\right)^{1/2}$ for a matrix whose i, j entry is A_{ij}.

Modulo isometries, distance is the only invariant of a pair of points, but triples have another invariant, known as the *Bargmann invariant* [13] or *shape invariant* [18]. In terms of projection matrices, it equals $\operatorname{Re}\operatorname{Tr}\left(\Pi_1 \Pi_2 \Pi_3\right)$, and the information it conveys is essentially the symplectic area of the corresponding geodesic triangle [60; 40]. One can define similar invariants for more than three points, but they can be computed in terms of three-point invariants as long as no two points are orthogonal. When no two points are orthogonal, the two- and three-point invariants characterize the entire configuration [19; 20].

The one remaining projective space we have not yet constructed is the octonionic projective plane $\mathbb{OP}^2$. (See [10] for an account of why $\mathbb{OP}^d$ cannot exist for $d > 2$; one can construct $\mathbb{OP}^1$, but we will ignore it as it is simply S^8.) Due to the failure of associativity, the construction of $\mathbb{OP}^2$ is more complicated than that of the other projective spaces; in particular, we cannot simply view it as the space of lines in $\mathbb{O}^3$. However, there is a construction analogous to the one using Hermitian matrices above. The result is an exceptionally beautiful space that has been called the panda of geometry [14, page 155]. The points of $\mathbb{OP}^2$ are 3×3 projection matrices over $\mathbb{O}$, in other words, 3×3 Hermitian matrices Π satisfying $\Pi^2 = \Pi$ and $\operatorname{Tr}\Pi = 1$. The (chordal) metric in $\mathbb{OP}^2$ is given by

$$\rho(\Pi_1, \Pi_2) = \frac{1}{\sqrt{2}} \|\Pi_1 - \Pi_2\|_F = \sqrt{1 - \langle \Pi_1, \Pi_2 \rangle}.$$

Each projection matrix Π is of the form

$$\Pi = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \begin{pmatrix} \bar{a} & \bar{b} & \bar{c} \end{pmatrix},$$

where $a, b, c \in \mathbb{O}$ satisfy $|a|^2 + |b|^2 + |c|^2 = 1$ and $(ab)c = a(bc)$. We can cover $\mathbb{OP}^2$ by three affine charts as follows. Any point may be represented by a triple

$(a,b,c) \in \mathbb{O}^3$ with $|a|^2+|b|^2+|c|^2=1$, and for the three charts we assume a, b or c are in $\mathbb{R}_+$, respectively. In practice, for computations with generic configurations we can simply work in the first chart and refer to a projection matrix by its associated point $(a,b,c) \in \mathbb{R}_+ \times \mathbb{O}^2$.

2.2 Tight simplices

Projective spaces can be embedded into Euclidean space by mapping each point to the corresponding projection matrix; using this embedding, the standard bounds on the size and distance of regular Euclidean simplices imply bounds on projective simplices. The resulting bounds, which we review in this subsection, were first proven by Lemmens and Seidel [54]. They are also known in information theory as Welch bounds [73].

As above, let K be $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ or $\mathbb{O}$. We consider regular simplices in $K\mathbb{P}^{d-1}$, with the understanding that $d=3$ when $K=\mathbb{O}$.

Definition 2.1 A *regular simplex* in a metric space (X,ρ) is a collection of distinct points $x_1,\dots,x_N$ of X with the distances $\rho(x_i,x_j)$ all equal for $i \neq j$.

We often drop the adjective "regular" and refer to a regular simplex as a simplex.

Proposition 2.2 *Consider a regular simplex in $K\mathbb{P}^{d-1}$ consisting of $N>1$ points $x_1,\dots,x_N$ with associated projection matrices $\Pi_1,\dots,\Pi_N$, and let $\alpha=\langle \Pi_i,\Pi_j\rangle$ be the common inner product for $i \neq j$. Then*

$$N \le d + \frac{(d^2-d)\dim_{\mathbb{R}} K}{2}$$

and, for any such value of N,

$$\alpha \ge \frac{N-d}{d(N-1)}.$$

Proof The Gram matrix G associated to $\Pi_1,\dots,\Pi_N$ has unit diagonal and α in each off-diagonal entry. Since G is nonsingular,[3] the elements $\Pi_1,\dots,\Pi_N \in \mathcal{H}(K^d)$ are linearly independent, implying $N \le \dim_{\mathbb{R}} \mathcal{H}(K^d) = d + (d^2-d)(\dim_{\mathbb{R}} K)/2$. Now note that $\langle \Pi_i, I_d\rangle = |x_i|^2 = 1$ for each $i=1,\dots,N$. Using this we compute

$$\left\langle \left(\sum_{i=1}^N \Pi_i\right) - \frac{N}{d} I_d, \left(\sum_{i=1}^N \Pi_i\right) - \frac{N}{d} I_d \right\rangle = N - \frac{N^2}{d} + N(N-1)\alpha.$$

Nonnegativity of this expression gives the desired bound on α. □

[3] Specifically, $G=(1-\alpha)I_N + \alpha v v^t$, where v is the all-ones vector, and therefore the eigenvalues of G are $1-\alpha$ (with multiplicity $N-1$) and $1+(N-1)\alpha$. These are all nonzero because $\alpha \in [0,1)$.

Definition 2.3 We refer to a regular simplex with

$$\alpha = \frac{N-d}{d(N-1)}$$

as a *tight simplex*. That is, it is a simplex with the maximum possible distance allowed by Proposition 2.2.

We noted above the difference between tight codes and tight designs, and on the surface Definition 2.3 seems to introduce a third notion of tightness. However, we will see that a tight simplex is a tight code (Lemma 2.9), so this new definition is really just a specialization.

Note that Definition 2.3 is independent of the coordinate algebra K. In other words, the canonical embeddings $\mathbb{RP}^{d-1} \hookrightarrow \mathbb{CP}^{d-1} \hookrightarrow \mathbb{HP}^{d-1}$ and $\mathbb{HP}^2 \hookrightarrow \mathbb{OP}^2$ preserve tight simplices.

It is not known for which N, d and K a tight simplex exists; later in this section we will survey the known examples. When $K = \mathbb{R}$, this problem is fundamentally combinatorial. Specifically, consider the Gram matrix of some corresponding unit vectors in $\mathbb{R}^d$. All the off-diagonal entries must be

$$\pm\sqrt{\frac{N-d}{d(N-1)}},$$

and the simplex is determined by the sign pattern. Thus, up to isometry, there can be only finitely many tight simplices of a given size in $\mathbb{RP}^{d-1}$. Furthermore, any sufficiently close numerical approximation will determine the signs and let one reconstruct the exact simplex.

By contrast, tight simplices are much more subtle when $K \neq \mathbb{R}$. The Gram matrix entries have phases, not just signs, and tight simplices can even occur in positive-dimensional families. In terms of the Bargmann invariants, the three-point invariants are not determined by the pairwise distances. No simple way to reconstruct an exact simplex from an approximation is known, and we see no reason to believe one exists.

Proposition 2.4 *Every tight simplex is an optimal code.*

More generally, the bound on α in Proposition 2.2 applies to the minimal distance of any code, not just a simplex.

Proof Let $\Pi_1, \dots, \Pi_N$ be the projection matrices corresponding to any N–point code in $K\mathbb{P}^{d-1}$. As in the proof of Proposition 2.2,

$$N - \frac{N^2}{d} + \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \langle \Pi_i, \Pi_j \rangle = \left\langle \left(\sum_{i=1}^{N} \Pi_i \right) - \frac{N}{d} I_d, \left(\sum_{i=1}^{N} \Pi_i \right) - \frac{N}{d} I_d \right\rangle \geq 0.$$

Thus, the average of $\langle \Pi_i, \Pi_j \rangle$ over all $i \neq j$ satisfies

$$\frac{1}{N(N-1)} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \langle \Pi_i, \Pi_j \rangle \geq \frac{N^2/d - N}{N(N-1)} = \frac{N-d}{d(N-1)}.$$

In particular, the greatest value of $\langle \Pi_i, \Pi_j \rangle$ for $i \neq j$ must be at least this large. □

A regular simplex of $N \leq d$ points in $K\mathbb{P}^{d-1}$ is optimal if and only if the points are orthogonal (in other words, $\alpha = 0$). Such simplices always exist. We only consider them to be tight when $N = d$, as the $N < d$ cases do not satisfy Definition 2.3; these degenerate cases are tight simplices in a lower-dimensional projective space. There also always exists a tight simplex with $N = d + 1$ points, obtained by projecting the regular simplex on the sphere S^{d-1} into $\mathbb{R}\mathbb{P}^{d-1}$. Therefore in what follows we will generally assume that $N \geq d + 2$.

It follows immediately from the proof of Proposition 2.2 that a regular simplex $\{x_1, \dots, x_N\}$ is tight if and only if

$$\sum_{i=1}^{N} x_i x_i^\dagger = \frac{N}{d} I_d.$$

This condition can be reformulated in the language of projective designs [34; 62]; see also [43] for a detailed account of the relevant computations in projective space. Specifically, it says that the configuration is a 1–design. We will make no serious use of the theory of designs in this paper, and for our purposes we could simply regard $\sum_{i=1}^{N} x_i x_i^\dagger = (N/d) I_d$ as the definition of a 1–design. However, to put our discussion in context, we will briefly recall the general concept of designs in the next subsection.

2.3 Linear programming bounds

Linear programming bounds [47; 34] use harmonic analysis on a space X to prove bounds on codes in X. These bounds and their extensions [9] are among the only known ways to prove systematic bounds on codes, and they are sharp in a number of important cases. Later in this section we summarize the sharp cases that are known in projective spaces (see also [29, Table 1] for a corresponding list for spheres), but first we give a brief review of how linear programming bounds work.

The simplest setting for linear programming bounds is a compact two-point homogeneous space. We will focus on the connected examples, namely spheres and projective spaces, but discrete two-point homogeneous spaces such as the Hamming cube are also important in coding theory.

Let X be a sphere or projective space, and let G be its isometry group under the geodesic metric ϑ (normalized so that the greatest distance is π). Then $L^2(X)$ is a unitary representation of G, and we can decompose it as a completed direct sum

$$L^2(X) = \widehat{\bigoplus_{k\geq 0}} V_k$$

of irreducible representations V_k. There is a corresponding sequence of *zonal spherical functions* $C_0, C_1, \dots$, one attached to each representation V_k. The zonal spherical functions are most easily obtained as reproducing kernels; for a brief review of the theory, see [29, Sections 2.2 and 8]. We can represent them as orthogonal polynomials with respect to a measure on $[-1,1]$, which depends on the space X, and we index the polynomials so that C_k has degree k.

For our purposes, the most important property of zonal spherical functions is that they are *positive-definite kernels*: for all $N \in \mathbb{N}$ and $x_1, \dots, x_N \in X$, the $N \times N$ matrix $(C_i(\cos\vartheta(x_i, x_j)))_{1\leq i,j\leq N}$ is positive semidefinite. In fact, the zonal spherical functions span the cone of all such functions.

For projective spaces $K\mathbb{P}^{d-1}$, the C_k may be taken to be the Jacobi polynomials $P_k^{(\alpha,\beta)}$, where $\alpha = \frac{1}{2}(d-1)\dim_{\mathbb{R}} K - 1$ (equivalently, $\alpha = \frac{1}{2}\dim_{\mathbb{R}} K\mathbb{P}^{d-1} - 1$) and $\beta = \frac{1}{2}\dim_{\mathbb{R}} K - 1$. We will normalize C_0 to be 1.

Linear programming bounds for codes amount to the following proposition.

Proposition 2.5 *Let $\theta \in [0,\pi]$, and suppose the polynomial*

$$f(z) = \sum_{k=0}^{n} f_k C_k(z)$$

satisfies $f_0 > 0$, $f_k \geq 0$ for $1 \leq k \leq n$, and $f(z) \leq 0$ for $-1 \leq z \leq \cos\theta$. Then every code in X with minimal geodesic distance at least θ has size at most $f(1)/f_0$.

Proof Let $\mathcal{C}$ be such a code. Then

$$\sum_{x,y\in\mathcal{C}} f(\cos\vartheta(x,y)) \geq f_0|\mathcal{C}|^2,$$

because each zonal spherical function C_k is positive definite and hence satisfies

$$\sum_{x,y\in\mathcal{C}} C_k(\cos\vartheta(x,y)) \geq 0.$$

On the other hand, $f(\cos\vartheta(x,y)) \leq 0$ whenever $\vartheta(x,y) \geq \theta$, and hence

$$\sum_{x,y\in\mathcal{C}} f(\cos\vartheta(x,y)) \leq |\mathcal{C}|f(1)$$

because only the diagonal terms contribute positively. It follows that $f_0|\mathcal{C}|^2 \leq f(1)|\mathcal{C}|$, as desired. $\square$

We say this bound is *sharp* if there is a code $\mathcal{C}$ with minimal distance at least θ and $|\mathcal{C}| = f(1)/f_0$. Note that we require exact equality, rather than just $|\mathcal{C}| = \lfloor f(1)/f_0 \rfloor$.

Definition 2.6 A *tight code* is one for which linear programming bounds are sharp.

Examining the proof of Proposition 2.5 yields the following characterization of tight codes.

Lemma 2.7 *A code $\mathcal{C}$ with minimal geodesic distance θ is tight if and only if there is a polynomial $f(z) = \sum_{k=0}^{n} f_k C_k(z)$ satisfying $f_0 > 0$, $f_k \geq 0$ for $1 \leq k \leq n$, $f(z) \leq 0$ for $-1 \leq z \leq \cos\theta$,*

$$\sum_{x,y\in\mathcal{C}} C_k(\cos\vartheta(x,y)) = 0$$

whenever $f_k > 0$ and $k \neq 0$, and $f(\cos\vartheta(x,y)) = 0$ for $x, y \in \mathcal{C}$ with $x \neq y$. In fact, these conditions must hold for every polynomial f satisfying both $f(1)/f_0 = |\mathcal{C}|$ and the hypotheses of Proposition 2.5.

By Proposition 2.5, every tight code is as large as possible given its minimal distance, but it is less obvious that such a code maximizes minimal distance given its size.

Proposition 2.8 *Every tight code is optimal.*

Proof Suppose f satisfies the hypotheses of Proposition 2.5, and $\mathcal{C}$ is a code of size $f(1)/f_0$ with minimal geodesic distance at least θ. We wish to show that its minimal distance is exactly θ.

By Lemma 2.7,

$$\sum_{x,y\in\mathcal{C}} (f(\cos\vartheta(x,y)) - f_0) = 0,$$

and $f(\cos\vartheta(x,y)) = 0$ for $x,\ y \in \mathcal{C}$ with $x \neq y$.

Now suppose $\mathcal{C}$ had minimal geodesic distance strictly greater than θ, and consider a small perturbation $\mathcal{C}'$ of $\mathcal{C}$. It must satisfy

$$\sum_{x,y\in\mathcal{C}'} (f(\cos\vartheta(x,y)) - f_0) \geq 0,$$

by positive definiteness. On the other hand,

$$\sum_{x,y\in\mathcal{C}'} (f(\cos\vartheta(x,y)) - f_0) = |\mathcal{C}'| f(1) - |\mathcal{C}'|^2 f_0 + \sum_{\substack{x,y\in\mathcal{C}'\\ x\neq y}} f(\cos\vartheta(x,y)).$$

We have $|\mathcal{C}'| f(1) - |\mathcal{C}'|^2 f_0 = 0$ since $|\mathcal{C}'| = |\mathcal{C}| = f(1)/f_0$. Thus,

$$\sum_{\substack{x,y\in\mathcal{C}'\\ x\neq y}} f(\cos\vartheta(x,y)) \geq 0.$$

If the perturbation is small enough, then the minimal distance of $\mathcal{C}'$ remains greater than θ and hence $f(\cos\vartheta(x,y)) \leq 0$ for distinct $x,\ y \in \mathcal{C}'$. In that case, we must have $f(\cos\vartheta(x,y)) = 0$ for distinct $x,\ y \in \mathcal{C}'$. However, this fails for some perturbations, for example if we move two points slightly closer together. It follows that every code of size $f(1)/f_0$ and minimal geodesic distance at least θ has minimal distance exactly θ, so these codes are all optimal. □

Lemma 2.9 *Tight simplices in projective space are tight codes.*

Proof Up to scaling, the first-degree zonal spherical function C_1 on $K\mathbb{P}^{d-1}$ is $z + (d-2)/d$. Now let

$$f(z) = 1 + \frac{(N-1)d}{2(d-1)}\Big(z + \frac{d-2}{d}\Big).$$

It satisfies $f(z) \leq 0$ for $z \in [-1, 2\alpha - 1]$, where

$$\alpha = \frac{N-d}{d(N-1)},$$

and $f(1)/f_0 = N$, as desired. □

Note that in this proof C_1 depends only on d, and not on K. By contrast, higher-degree zonal spherical functions for $K\mathbb{P}^{d-1}$ depend on both d and K.

We have no proof that every tight N–point code in $K\mathbb{P}^{d-1}$ with

$$d \leq N \leq d + \frac{(d^2-d)\dim_{\mathbb{R}} K}{2}$$

is a tight simplex, although we know of no counterexample. This assertion would follow if the linear function $f(z)$ from the proof of Lemma 2.9 always gave the optimal bound for this range of N, but it does not. For example, consider 5–point codes in $\mathbb{RP}^2$, with $d=3$, $K=\mathbb{R}$, $N=5$. If there were a tight simplex with these parameters, then it would have common squared inner product $\alpha=\frac{1}{6}$, and positive definiteness of C_k would require that $C_k(1)+4C_k\big(2\cdot\frac{1}{6}-1\big)\geq 0$ for all k. However, $C_4(1)+4C_4\big(-\frac{2}{3}\big)<0$. This means that no tight simplex exists, and, in terms of linear programming bounds,[4] it means that we can improve on the linear function $f(z)$ by replacing it with $f(z)+\varepsilon\big(C_4(z)-C_4\big(-\frac{2}{3}\big)\big)$, for small positive ε.

A *t–design* in X is a code $\mathcal{C}\subset X$ such that for every $f\in V_k$ with $0<k\leq t$,

$$\sum_{x\in\mathcal{C}} f(x)=0.$$

In other words, every element of $V_0\oplus\cdots\oplus V_t$ has the same average over $\mathcal{C}$ as over the entire space X. (Note that all functions in V_k for $k>0$ have average zero, since they are orthogonal to the constant functions in V_0.) Using the reproducing kernel property, this can be shown to be equivalent to

$$\sum_{x,y\in\mathcal{C}} C_k(\cos\vartheta(x,y))=0$$

for $0<k\leq t$.

In $K\mathbb{P}^{d-1}$, one can check that

$$\sum_{i=1}^{N} x_i x_i^\dagger=\frac{N}{d}I_d$$

holds if and only if $\{x_1,\dots,x_N\}$ is a 1–design.

A code is *diametrical* in X if it contains two points at maximal distance in X, and it is an *m–distance set* if exactly m distances occur between distinct points.

Definition 2.10 A *tight design* is an m–distance set that is a $(2m-\varepsilon)$–design, where ε is 1 if the set is diametrical and 0 otherwise.

For example, an N–point tight simplex in $K\mathbb{P}^{d-1}$ with $N=d+(d^2-d)(\dim_{\mathbb{R}} K)/2$ (the largest possible value of N) is a tight 2–design. See [12] for further examples.

[4] In fact, linear programming bounds prove a bound of $0.16866\ldots$ (a cubic irrational) for the maximal squared inner product of any 5–point code in $\mathbb{RP}^2$. This bound is not achieved by any real code, so in particular there is no tight 5–point code, simplex or otherwise.

Every tight t–design is the smallest possible t–design in its ambient space. This was first proved for spheres in [34]; see [11, Propositions 1.1 and 1.2] for the general case. The converse is false: the smallest t–design is generally not tight.

A theorem of Levenshtein [56] says that every m–distance set that is a $(2m-1-\varepsilon)$–design is a tight code, where as above ε is 1 if the set is diametrical and 0 otherwise. For example, all tight designs are tight codes. In [29], it was also shown that under these conditions, $\mathcal{C}$ is *universally optimal* for potential energy: it minimizes energy for every completely monotonic function of squared chordal distance. (See also [28] for context.) This applies in particular to simplices, so all tight simplices are universally optimal.

In fact every known tight code is universally optimal. Moreover, except for the regular 600–cell in S^3 and its image in $\mathbb{RP}^3$, they all satisfy the design condition just mentioned. For lack of a counterexample, we conjecture that tight codes are always universally optimal. (But see [30] for perspective on why the simplest reason why this might hold fails.)

2.4 Tight codes in $\mathbb{RP}^{d-1}$

We now describe what is known about tight codes in real projective spaces. Table 1 provides a summary of the current state of knowledge. Note that in several lines in the table, existence of a code is conditional on existence of a combinatorial object such as a conference matrix; we provide further details in the text below. See also [72, Table 1], which provides a list of all known tight simplices in $\mathbb{RP}^{d-1}$ with $d \le 50$ and all cases in this range that have not been resolved.

Euclidean simplices and orthogonal points give the simplest infinite families of tight codes.

Another infinite family of tight simplices comes from conference matrices [57] (see [31, page 156]): if a symmetric conference matrix of order $2d$ exists, then there is a tight simplex of size $2d$ in $\mathbb{R}^d$. In particular, we get a tight simplex in $\mathbb{R}^d$ whenever $2d-1$ is a prime power congruent to 1 modulo 4. One can also construct such codes through the Weil representation of the group $G = \mathrm{PSL}_2(\mathbb{F}_q)$. Note that the icosahedron arises as the special case $q = 5$, which is why it is not listed separately in Table 1.

Levenshtein [55] described a family of tight codes in $\mathbb{RP}^{d-1}$ for d a power of 4, based on a construction using Kerdock codes; the regular 24–cell is the special case with $d = 4$. These codes meet the orthoplex bound [31, Corollary 5.3] and give rise to $d/2+1$ mutually unbiased bases in their dimensions. Recall that two orthonormal

d	N	$\max\lvert\langle x, y\rangle\rvert^2$	Name/origin
d	$N \le d$	0	orthogonal points (tight when $N = d$)
d	$d+1$	$*$	Euclidean simplex
d	$2d$	$*$	symm. conf. matrix of order $2d$ $(\star)$
d	$d(d+2)/2$	$1/d$	$d/2+1$ mutually unbiased bases $(\star)$
2	N	$\cos^2(\pi/N)$	regular polygon
4	60	$(\sqrt{5}-1)/4$	regular 600–cell
6	16	$*$	Clebsch
6	36	$1/4$	E_6 root system
7	28	$*$	equiangular lines
7	63	$1/4$	E_7 root system
8	120	$1/4$	E_8 root system
23	276	$*$	equiangular lines
23	2300	$1/9$	kissing configuration of next line
24	98280	$1/4$	Leech lattice minimal vectors
$\frac{v(v-1)}{k(k-1)}$	$v\bigl(1+\frac{v-1}{k-1}\bigr)$	$*$	Steiner construction $(\star)$
d	N	$*$	strongly regular graph with parameters $(N-1, k, (3k-N)/2, k/2)$, where $k = \frac{N}{2} - 1 + \bigl(1 - \frac{N}{2d}\bigr)\sqrt{\frac{d(N-1)}{N-d}}$ $(\star)$

Table 1: Known universal optima of N points in real projective spaces $\mathbb{RP}^{d-1}$. The tight simplices are indicated by an asterisk in the third column and have maximal squared inner product $(N-d)/(d(N-1))$; for brevity we omit the Gale duals of the tight simplices. A star in the last column means the code may exist only for certain parameter settings.

bases $v_1, \dots, v_d$ and $w_1, \dots, w_d$ are *mutually unbiased* if $|\langle v_i, w_j\rangle|^2 = 1/d$ for all i and j.

A trivial systematic family of tight codes is formed by the diameters of the regular polygons in the plane. The next nine lines in Table 1 correspond to exceptional geometric structures.

The Steiner construction from [36] builds a tight simplex from a $(2, k, v)$ Steiner system and a Hadamard matrix of order $1 + (v-1)/(k-1)$. See [36] for a discussion of the parameters that can be achieved using different sorts of Steiner systems. (Note that Bondarenko's tight simplex [15] is a Steiner simplex with $(k, v) = (3, 15)$.) Steiner simplices can be constructed as follows. Recall that a $(2, k, v)$ Steiner system is a set of v points with a collection of subsets of size k called blocks, such that every two distinct points belong to a unique block. Then there must be d blocks, and every point is in r blocks, where

$$d = \frac{v(v-1)}{k(k-1)} \quad \text{and} \quad r = \frac{v-1}{k-1}.$$

Consider the $d \times v$ incidence matrix A for blocks and points, with entries 0 and 1, and let H be a Hadamard matrix of order $r+1$. For each j from 1 to v, consider the j^{th} column of A, and form a $d \times (r+1)$ matrix M_j whose i^{th} row is a different row of H for each i satisfying $A_{i,j} \neq 0$ and vanishes otherwise. Then it is not difficult to check that the $v(1+r)$ columns of all these matrices M_j form a tight simplex in $\mathbb{RP}^{d-1}$.

The last entry in the table is a reformulation of tight simplices in $\mathbb{RP}^{d-1}$ in terms of strongly regular graphs; see [72, Theorem 5.2]. This sort of combinatorial description works only over the real numbers. When $d \leq 50$, only three cases are known that are not encompassed by other lines in the table: $(d, N) = (22, 176)$, $(36, 64)$ and $(43, 344)$. See [72, Table 1] for more information.

We also observe the phenomenon of Gale duality: tight simplices of size N in $K\mathbb{P}^{d-1}$ correspond to tight simplices of size N in $K\mathbb{P}^{N-d-1}$. For instance, the Gale dual of the Clebsch configuration gives a tight simplex of 16 points in $\mathbb{RP}^9$. See Section 2.7 for more details.

2.5 Tight codes in $\mathbb{CP}^{d-1}$

Table 2 lists the tight codes we are aware of in complex projective spaces. For a detailed survey of tight simplices, we refer the reader to [50, Chapter 4].

Here, we observe a few more infinite families. In particular, if a conference matrix of order $2d$ exists, then there is a tight code of $2d$ lines in $\mathbb{CP}^{d-1}$ [76, page 66]. For prime powers $q \equiv 3 \pmod 4$, this gives a construction of a tight $(q+1)$–point code in $\mathbb{CP}^{(q-1)/2}$. As mentioned before, such codes may also be constructed using the Weil representation of $\mathrm{PSL}_2(\mathbb{F}_q)$. Another family of codes of $d(d+1)$ points in $\mathbb{CP}^{d-1}$, for d an odd prime power, was constructed by Levenshtein [55] using dual BCH codes. These codes meet the orthoplex bound and give rise to $d+1$ mutually unbiased bases in their dimensions. They were rediscovered by Wootters and Fields [74], with an extension to characteristic 2 and applications to physics. A third infinite family is obtained from skew-Hadamard matrices (see [66] for a construction using

d	N	$\max\lvert\langle x, y\rangle\rvert^2$	Name/origin
d	$2d$	$*$	skew-symm. conf. matrix of order $2d$ $(\star)$
d	d^2	$*$	SIC-POVMs $(\star)$
d	$d(d+1)$	$1/d$	$d+1$ mutually unbiased bases $(\star)$
$2k-1$	$4k-1$	$*$	skew-Hadamard matrix of order $4k$ $(\star)$
$2k$	$4k-1$	$*$	skew-Hadamard matrix of order $4k$ $(\star)$
4	40	$1/3$	Eisenstein structure on E_8
5	45	$1/4$	kissing configuration of next line
6	126	$1/4$	Eisenstein structure on K_{12}
28	4060	$1/16$	Rudvalis group
$\frac{v(v-1)}{k(k-1)}$	$v\bigl(1+\frac{v-1}{k-1}\bigr)$	$*$	Steiner construction $(\star)$
$\lvert S\rvert$	$\lvert G\rvert$	$*$	difference set S in abelian group G $(\star)$

Table 2: Known universal optima of N points in complex projective spaces $\mathbb{CP}^{d-1}$. The tight simplices are indicated by an asterisk in the third column and have maximal squared inner product $(N-d)/(d(N-1))$; for brevity we omit the Gale duals of the tight simplices as well as the tight simplices from $\mathbb{RP}^{d-1}$. A star in the last column means the code may exist only for certain parameter settings.

explicit families of skew-Hadamard matrices and [50, Theorem 4.14] for the general case).

The most mysterious tight simplices are the awkwardly named SIC-POVMs (symmetric, informationally complete, positive operator-valued measures). SIC-POVMs are simplices of size d^2 in $\mathbb{CP}^{d-1}$, that is, simplices of the greatest size allowed by Proposition 2.2. These configurations play an important role in quantum information theory, which leads to their name. Numerical experiments suggest they exist in all dimensions, and that they can even be taken to be orbits of the Weyl–Heisenberg group [76; 67]. Exact SIC-POVMs are known for $d \le 16$, as well as $d = 19$, 24, 28, 35 and 48, while numerical approximations are known for all $d \le 67$ (see [69] and [3]).

The Steiner construction can be carried out in $\mathbb{CP}^{d-1}$ using a complex Hadamard matrix instead of a real Hadamard matrix (see [36]). Complex Hadamard matrices of every order exist, so the construction applies whenever there is a $(2,k,v)$ Steiner system.

The last line of the table refers to a construction based on difference sets [75] (see also [51]). Let G be an abelian group of order N, let S be a subset of G of order d, and let λ be a natural number such that every nonzero element of G is a difference of exactly λ pairs of elements of S. It follows that $d(d-1) = \lambda(N-1)$, and that the vectors

$$v_\chi = (\chi(s))_{s\in S}$$

give rise to a tight simplex of N points in $\mathbb{P}^{d-1}$ as χ ranges over all characters of G. As particular cases of this construction, one can obtain a tight simplex of n^2+n+1 points in $\mathbb{CP}^n$ when there is a projective plane of order n. A generalization of this example was given in [75], using Singer difference sets, to produce $(q^{d+1}-1)/(q-1)$ points in $\mathbb{CP}^{d-1}$, with $d=(q^d-1)/(q-1)$. Similarly, if q is a prime power congruent to 3 modulo 4, then the quadratic residues give a difference set, yielding a tight simplex of q points in $\mathbb{CP}^{(q-3)/2}$. As another example, there is a difference set of 6 points in $\mathbb{Z}/31\mathbb{Z}$ (namely, $\{0,1,4,6,13,21\}$), which gives rise to a tight simplex of 31 points in $\mathbb{CP}^5$.

2.6 Tight codes in $\mathbb{HP}^{d-1}$ and $\mathbb{OP}^2$

Space	N	$\max\lvert\langle x,y\rangle\rvert^2$	Name/origin
$\mathbb{HP}^{d-1}$	$d(2d+1)$	$1/d$	$2d+1$ mutually unbiased bases $(\star)$
$\mathbb{HP}^4$	165	$1/4$	quaternionic reflection group
$\mathbb{OP}^2$	819	$1/2$	generalized hexagon of order $(2,8)$

Table 3: Previously known universal optima of N points in quaternionic and octonionic projective spaces. For brevity we omit the tight simplices from $\mathbb{RP}^{d-1}$ and $\mathbb{CP}^{d-1}$. A star in the last column means the code may exist only for certain parameter settings.

Relatively little is known about tight codes in quaternionic or octonionic projective spaces, aside from the real and complex tight simplices they automatically contain. When d is a power of 4, there is a construction of $2d+1$ mutually unbiased bases in $\mathbb{HP}^{d-1}$ due to Kantor [48], and two exceptional codes are known.

The 165 points in $\mathbb{HP}^4$ from Table 3 are constructed using a quaternionic reflection group [43, Example 9]. The 819–point universal optimum is a remarkable code in the octonionic projective plane [27]; see also [35] for another construction. It can be thought of informally as the 196560 Leech lattice minimal vectors modulo the action of the 240 roots of E_8 (viewed as units in the integral octonions), although this does not yield an actual construction: there is no such action because the multiplication is not associative.

2.7 Gale duality

Gale duality is a fundamental symmetry of tight simplices. It goes by several names in the literature, such as coherent duality, Naimark complements and the theory of eutactic stars. We call it Gale duality because it is a metric version of Gale duality from the theory of polytopes (see [71, Chapter 5] for the non-metric Gale transform).

Let K be $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. (Gale duality does not apply to $\mathbb{O}\mathbb{P}^2$.)

Proposition 2.11 (Hadwiger [39]) *Let $v_1, \dots, v_N$ span a d–dimensional vector space V over K, and suppose they have the same norm $|v_i|^2 = d/N$. Then their images in $K\mathbb{P}^{d-1}$ form a 1–design if and only if there is an N–dimensional vector space U containing V and an orthonormal basis $u_1, \dots, u_N$ of U such that v_i is the orthogonal projection of u_i to V.*

Proof Let M be the $d \times N$ matrix whose i^{th} column is v_i. The existence of U and $u_1, \dots, u_N$ is equivalent to that of an extension of M to a unitary matrix by adding $N - d$ rows, in which case $u_1, \dots, u_N$ are the columns of the extended matrix. This extension is possible if and only if the rows of M are orthonormal vectors; in other words, it is equivalent to $MM^\dagger = I_d$.

To analyze M, we can write it as $M = \sum_{i=1}^N v_i e_i^\dagger$, where $e_1, \dots, e_N$ is the standard orthonormal basis of K^N. Then

$$MM^\dagger = \sum_{i,j=1}^N v_i e_i^\dagger e_j v_j^\dagger = \sum_{i=1}^N v_i v_i^\dagger.$$

Thus, the extension is possible if and only if

$$\sum_{i=1}^N v_i v_i^\dagger = I_d.$$

This equation is the condition for a projective 1–design once we rescale to account for the normalization $|v_i|^2 = d/N$. □

Under the 1–design condition from Proposition 2.11, consider the projections w_i of the vectors u_i to the orthogonal complement $V^\perp$ of V in U. This code $\{w_1, \dots, w_N\}$ in $K\mathbb{P}^{N-d-1}$ is called the *Gale dual* of the code $\{v_1, \dots, v_N\}$ in $K\mathbb{P}^{d-1}$. The construction from the proof shows that the Gale dual is well defined up to unitary transformations of $V^\perp$. However, there is one technicality: the N points in $K\mathbb{P}^{N-d-1}$ need not be distinct in general, so the Gale dual must be considered a multiset of points.

Aside from the need to allow multisets, Gale duality is an involution on projective 1–designs, defined up to isometry.

Gale duality preserves tight simplices when $N > d+1$, and the multiplicity issue does not arise:

Corollary 2.12 *Let K be $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. For $N > d+1$, the Gale dual of an N–point tight simplex in $K\mathbb{P}^{d-1}$ is an N–point tight simplex in $K\mathbb{P}^{N-d-1}$.*

Proof Because the 1–design property is preserved, we need only check that the Gale dual is a simplex. In the notation used above, for $i \neq j$ we have

$$0 = \langle u_i, u_j \rangle = \langle v_i, v_j \rangle + \langle w_i, w_j \rangle.$$

Thus, $\langle w_i, w_j \rangle$ is constant for $i \neq j$ because $\langle v_i, v_j \rangle$ is. The inequality $N > d+1$ merely rules out the degenerate case $K\mathbb{P}^0$. □

The inequality

$$N \le d + \frac{(d^2-d)\dim_{\mathbb{R}} K}{2}$$

from Proposition 2.2 shows that tight simplices cannot be too large. Combining Gale duality with the same inequality shows that they cannot be too small either (see [76, Theorem 2.30] and [50, Corollary 2.19]):

Corollary 2.13 *Let K be $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. If there exists an N–point tight simplex in $K\mathbb{P}^{d-1}$ with $N > d+1$, then*

$$N \ge d + \frac{1+\sqrt{1+8d/(\dim_{\mathbb{R}} K)}}{2}.$$

3 Effective existence theorems

Our main tool is an effective implicit function theorem, which gives conditions under which an approximate solution to a system of equations necessarily leads to a nearby exact solution. Theorems of this sort date back to the Newton–Kantorovich theorem [49] on the convergence of Newton's method (see also [63] for a short proof). Our formulation is closer to Krawczyk's version of Newton–Kantorovich [53], but it differs in that we focus on existence of solutions rather than convergence of numerical algorithms.

The following theorem is a variant of [61, Theorem 2], and we adapt the proof given there. In the statement, $\|\cdot\|$ denotes the operator norm, $Df(x)$ is the Jacobian of f

at x, $B(x_0, \varepsilon)$ is the open ball around x_0 with radius ε, and id_W is the identity operator on W.

Theorem 3.1 *Let V and W be finite-dimensional normed vector spaces over $\mathbb{R}$, and suppose that $f\colon B(x_0, \varepsilon) \to W$ is a C^1 function, where $x_0 \in V$ and $\varepsilon > 0$. Suppose also that $T\colon W \to V$ is a linear operator such that*

$$\|Df(x) \circ T - \mathrm{id}_W\| < 1 - \frac{\|T\| \cdot |f(x_0)|}{\varepsilon} \tag{3-1}$$

for all $x \in B(x_0, \varepsilon)$. Then there exists an $x_* \in B(x_0, \varepsilon)$ such that $f(x_*) = 0$. Moreover, in $B(x_0, \varepsilon)$, the zero locus $f^{-1}(0)$ is a C^1 submanifold of dimension $\dim V - \dim W$.

Of course, the submanifold is smooth if f is C^∞.

Proof Consider the initial value problem

$$x'(t) = -T(Df(x(t)) \circ T)^{-1} f(x_0), \qquad x(0) = x_0, \tag{3-2}$$

which is a rescaling of the differential equation for the continuous analogue of Newton's method [61, Section 3]. The motivation is that

$$\begin{aligned}\frac{d}{dt}[f(x(t))] &= Df(x(t))(x'(t))\\ &= -(Df(x(t)) \circ T)(Df(x(t)) \circ T)^{-1} f(x_0)\\ &= -f(x_0),\end{aligned}$$

and so $f(x(t)) = (1-t) f(x_0)$. Thus, $x(1)$ should be a root of f, but of course we must verify that the initial value problem has a solution defined on [0, 1].

First note that the bound (3-1) implies that $Df(x) \circ T$ is invertible for all $x \in B(x_0, \varepsilon)$. Moreover, supposing for the moment that $f(x_0) \neq 0$, we have

$$\|(Df(x) \circ T)^{-1}\| < \frac{\varepsilon}{\|T\| \cdot |f(x_0)|}. \tag{3-3}$$

These claims follow from the series expansion

$$(Df(x) \circ T)^{-1} = \sum_{i=0}^{\infty} (\mathrm{id}_W - Df(x) \circ T)^i.$$

Because f is C^1, $(Df(x) \circ T)^{-1}$ is continuous. Thus, by the Peano existence theorem [26, Chapter 1, Sections 1–5], the initial value problem (3-2) has a C^1 solution $x(t)$

defined on a nontrivial interval starting at 0. The solution can be extended as long as $x(t)$ does not approach the boundary of $B(x_0,\varepsilon)$. Using (3-3), we have

$$|x'(t)| \le \|T\| \cdot \|(Df(x(t)) \circ T)^{-1}\| \cdot |f(x_0)| < \varepsilon.$$

It follows that the solution $x(t)$ can be continued to $t=1$ and satisfies $|x(t)-x_0| < \varepsilon t$. Setting $x_* = x(1)$ finishes the first part of the theorem.

Of course, if $f(x_0)=0$, then we can just take $x_* = x_0$.

It remains only to show that $f^{-1}(0)$ is a manifold of dimension $\dim V - \dim W$. We noted above that the operator $Df(x)\circ T$ is invertible for all $x \in B(x_0,\varepsilon)$, so in particular this is true for all $x \in f^{-1}(0)$. But that implies that $Df(x)$ is surjective, so we are done by an application of the standard implicit function theorem (see [52, Section 4.3]). □

Given a function f and an approximate root x_0, it is straightforward to apply this theorem. We must compute an approximate right inverse T of $Df(x_0)$ and bound $\|Df(x)\circ T - \mathrm{id}_W\|$ for all $x \in B(x_0,\varepsilon)$. The simplest and most elegant way to do this is using interval arithmetic (see Section 7 for details), but we can also use Corollary 3.4 below when f is a polynomial.

In order for Theorem 3.1 to prove the existence of a solution of $f(x)=0$, $Df(x)$ must have a right inverse at that solution. (In particular, we must have $\dim V \ge \dim W$.) If we view f as defining a system of simultaneous equations, then choosing the right equations to use can be tricky. For example, some of the most straightforward systems defining a tight simplex will not work to prove existence of such a simplex, because Df is singular at every solution. Much of this paper is devoted to formulating suitable systems defining different sorts of tight simplices. The generic cases are reasonably straightforward, but even they must be handled carefully, and a few extreme cases are particularly subtle (Propositions 4.11 and 5.8).

In our applications, f will always be a polynomial map. In this case, the following lemma can be useful in conjunction with Theorem 3.1.

Definition 3.2 For a polynomial $p\colon \mathbb{R}^m \to \mathbb{R}$ given by $p(x) = \sum_I c_I x^I$, define $|p| = \sum_I |c_I|$. Given a polynomial map $p=(p_1,\dots,p_n)\colon \mathbb{R}^m \to \mathbb{R}^n$, define $|p| = \max |p_i|$.

Lemma 3.3 *Let $m \ge n$, $\varepsilon > 0$, and $x_0 \in \mathbb{R}^m$. Suppose $f\colon \mathbb{R}^m \to \mathbb{R}^n$ is a polynomial function of total degree d, and let $\mathbb{R}^m$ and $\mathbb{R}^n$ carry the ℓ_∞ norm. Set $\eta = \max(1, |x_0|+\varepsilon)$. Then for all $x \in B(x_0,\varepsilon)$,*

$$\|Df(x) - Df(x_0)\| < |f|\, d(d-1)\varepsilon\eta^{d-2}.$$

Proof The $\ell_\infty \to \ell_\infty$ operator norm of a matrix is the maximum of the ℓ_1 norms of its rows, so we need to bound the ℓ_1 norm of each row of $Df(x) - Df(x_0)$. Without loss of generality suppose $n = 1$; in other words, work with a fixed row of the matrix. The quantity we want to bound is

$$A = \sum_{i=1}^{m} |\partial_i f(x) - \partial_i f(x_0)|,$$

where $\partial_i f$ denotes the partial derivative of f with respect to the i^{th} coordinate. Splitting this as a sum over the monomials of f, it suffices, by the triangle inequality, to prove that $A < e(e-1)\varepsilon\eta^{e-2}$ when f is a (monic) monomial of total degree $e \le d$. Using the mean value theorem applied to the function $g(t) = \partial_i f(x_0 + t(x - x_0))$, we have

$$\partial_i f(x) - \partial_i f(x_0) = \sum_{j=1}^{m} \partial_{ij}^2 f(v_i)(x - x_0)_j$$

for some v_i on the line segment between x_0 and x (where $(x - x_0)_j$ denotes the j^{th} coordinate of the vector $x - x_0$). Therefore,

$$A \le \sum_{i=1}^{m} \left| \sum_{j=1}^{m} \partial_{ij}^2 f(v_i)(x - x_0)_j \right| < \varepsilon \sum_{i,j=1}^{m} |\partial_{ij}^2 f(v_i)|,$$

since the ℓ_∞ norm $|x - x_0|$ is bounded by ε. Write $f = \prod_{k=1}^{m} x_k^{e_k}$. Then $\partial_{ij}^2 f(v_i)$ equals a monomial of degree $e-2$ times either $e_i e_j$ if $i \ne j$, or $e_i(e_i - 1)$ if $i = j$. Because $\eta \ge \max(|v_i|, 1)$, the monomial is bounded by η^{e-2}. Summing, we obtain

$$A < \varepsilon\eta^{e-2}\left(\sum_{i,j=1}^{m} e_i e_j - \sum_{i=1}^{m} e_i \right) = \varepsilon\eta^{e-2} e(e-1),$$

as desired. $\square$

Corollary 3.4 *Using the notation of Lemma 3.3, if there exists a linear operator $T\colon \mathbb{R}^n \to \mathbb{R}^m$ such that*

$$\| Df(x_0) \circ T - \mathrm{id}_{\mathbb{R}^n} \| + \varepsilon\, |f|\, d(d-1)\eta^{d-2} \|T\| < 1 - \frac{\|T\| \cdot |f(x_0)|}{\varepsilon},$$

then there exists an $x_* \in B(x_0, \varepsilon)$ such that $f(x_*) = 0$, and the zero locus $f^{-1}(0)$ is locally a manifold of dimension $m - n$.

Proof Using

$$\|Df(x)\circ T-\mathrm{id}_{\mathbb{R}^n}\|\leq\|Df(x)-Df(x_0)\|\cdot\|T\|+\|Df(x_0)\circ T-\mathrm{id}_{\mathbb{R}^n}\|,$$

we see that the hypotheses of Theorem 3.1 are met. □

4 Simplices in quaternionic projective spaces

4.1 Generic case

The definition gives one characterization of tight N–point simplices; we simply impose $|x_i|^2 = 1$ for each i and $|\langle x_i, x_j\rangle|^2 = (N-d)/(d(N-1))$ for $i < j$. In fact, tight simplices can be characterized even more succinctly: it can be shown that $\sum_{i,j}|\langle x_i, x_j\rangle|^2 \geq N^2/d$, with equality if and only if $\{x_1,\ldots,x_N\}$ is a tight simplex. Both of these descriptions, though, suffer from the problem that the imposed conditions are *singular*; loosely put, if a set of points satisfies the conditions, then it does so "just barely". For instance, if we define $f\colon \mathbb{H}^N \to \mathbb{R}^{N+1}$ by

$$f(x_1,\ldots,x_N)=\Big(|x_1|^2-1,\ldots,|x_N|^2-1,\sum_{i,j}|\langle x_i,x_j\rangle|^2-N^2/d\Big),$$

then the fact that the last coordinate is always nonnegative implies that the last row of Df is zero at a tight simplex. Therefore it is hopeless to try to prove existence by applying Theorem 3.1. Setting all the inner products equal to $(N-d)/(d(N-1))$ suffers from the same problem, because

$$\frac{1}{N(N-1)}\sum_{\substack{i,j=1\\ i\neq j}}^{N}|\langle x_i,x_j\rangle|^2\geq\frac{N-d}{d(N-1)}$$

for all $x_1,\ldots,x_N$ (see the proof of Proposition 2.4).

Fortunately, it is generally possible to recast the conditions describing tight simplices so that the Jacobian of the associated polynomial map becomes surjective.

Proposition 4.1 *Suppose $x_1,\ldots,x_N \in \mathbb{H}^d$ (for $d > 1$) and $w_1,\ldots,w_N \in \mathbb{R}$ satisfy the following conditions:*

(a) $|x_i|^2 = 1$ *for* $i = 1,\ldots,N$,

(b) $|\langle x_i, x_j\rangle|^2 = |\langle x_{i'}, x_{j'}\rangle|^2$ *for* $1 \leq i < j \leq N$ *and* $1 \leq i' < j' \leq N$, *and*

(c) $\sum_{i=1}^N w_i x_i x_i^\dagger = I_d$.

Then $w_1 = \cdots = w_N = d/N$ and $\{x_1,\ldots,x_N\}$ is a tight simplex in $\mathbb{HP}^{d-1}$.

Proof Define $\Pi_i = x_i x_i^\dagger$, and let α denote the common inner product $|\langle x_i, x_j\rangle|^2$ for $i \neq j$. By the first condition we have $\langle \Pi_i, I_d\rangle = 1$ for each i. Thus,

$$d = \langle I_d, I_d\rangle = \sum_{i=1}^{N} w_i \langle \Pi_i, I_d\rangle = \sum_{i=1}^{N} w_i.$$

Moreover, by (2-1) we have $\langle \Pi_i, \Pi_i\rangle = 1$ and $\langle \Pi_i, \Pi_j\rangle = \alpha$ for all $i \neq j$. Thus, for any j,

$$1 = \langle \Pi_j, I_d\rangle = \sum_{i=1}^{N} w_i \langle \Pi_j, \Pi_i\rangle = (1-\alpha) w_j + \alpha \cdot \sum_{i=1}^{N} w_i = (1-\alpha) w_j + \alpha d.$$

It follows that $w_j = (1-\alpha d)/(1-\alpha)$ for each j. Substituting back into the equation $\sum_{i=1}^{N} w_i = d$ yields $\alpha = (N-d)/(d(N-1))$, from which the result follows. □

Using Proposition 4.1, we can view tight simplices of N points in $\mathbb{HP}^{d-1}$ as the solutions of a system of

$$N + \left(\frac{N(N-1)}{2} - 1\right) + (2d^2 - d)$$

real constraints in

$$N(4d+1)$$

real variables. In situations where Theorem 3.1 applies to this system, we get a solution space of dimension (number of variables) – (number of constraints). This separately counts each unit-norm lift of the N elements of $\mathbb{HP}^{d-1}$, so the space of simplices has codimension $3N$. Moreover, the space of simplices is invariant under the action of the symmetry group of $\mathbb{HP}^{d-1}$, and we are most interested in the quotient, which is the moduli space of simplices. This symmetry group, the compact symplectic group $\mathrm{Sp}(d)$ (strictly speaking, modulo its center $\{\pm 1\}$), has real dimension $d(2d+1)$. Thus the actual dimension of the moduli space of simplices, local to this particular solution, is at least

$$r(N, \mathbb{HP}^{d-1}) := (4d-3)N - \frac{N(N-1)}{2} - 4d^2 + 1 \tag{4-1}$$

when Theorem 3.1 and Proposition 4.1 apply. Equality holds if the simplices in this neighborhood have finite stabilizers (in which case the moduli space of simplices is locally an orbifold of the desired dimension); in any case, the moduli space always has dimension at least $r(N, \mathbb{HP}^{d-1})$.

The discussion above is informal in the case of a positive-dimensional stabilizer, but it is not difficult to make the lower bound rigorous for topological dimension. Specifically, the solution space $\mathfrak{X}$ of the system of equations from Proposition 4.1 is a compact metric space, and locally a manifold of dimension $r(N, \mathbb{HP}^{d-1}) + 3N + \dim \mathrm{Sp}(d)$ near the solution we find. Thus its topological dimension is at least that large. The moduli space is $\mathfrak{X}/G$, where $G = \mathrm{Sp}(1)^N \times \mathrm{Sp}(d)$. Because G is compact, the quotient map $\mathfrak{X} \to \mathfrak{X}/G$ is closed and $\mathfrak{X}/G$ is Hausdorff. Thus, we can apply topological dimension theory for separable metric spaces to conclude that

$$\dim(\mathfrak{X}/G) \geq \dim \mathfrak{X} - \dim G \geq r(N, \mathbb{HP}^{d-1}),$$

as desired (see [46, Theorem VI 7, page 91]).

Note that Gale duality, which replaces d with $N-d$, preserves $r(N, \mathbb{HP}^{d-1})$, as one would expect. Furthermore, because $r(N, \mathbb{HP}^{d-1})$ is quadratic in N, it is also symmetric about the midpoint of the range in which it is positive. Specifically, $r(N, \mathbb{HP}^{d-1}) = r(8d-5-N, \mathbb{HP}^{d-1})$.

While a priori it is possible to have tight simplices of up to $N = 2d^2 - d$ points, we only have $r(N, \mathbb{HP}^{d-1}) \geq 0$ for N between roughly $(4-2\sqrt{2})d$ and $(4+2\sqrt{2})d$. That does not rule out larger tight simplices, but it does mean that this approach using Proposition 4.1 and Theorem 3.1 could not prove their existence. We believe that outside of this range, only sporadic examples will exist in general, but we conjecture that tight simplices always exist within the range where $r(N, \mathbb{HP}^{d-1}) \geq 0$, at least if one stays away from the boundary:

Conjecture 4.2 *As $d \to \infty$, there exist tight N–point simplices in $\mathbb{HP}^{d-1}$ for all N satisfying*

$$(4-2\sqrt{2}+o(1))d \leq N \leq (4+2\sqrt{2}-o(1))d.$$

Remark 4.3 We emphasize that $r(N, \mathbb{HP}^{d-1})$ is *defined* by (4-1). The assertion that the moduli space of simplices locally has dimension $r(N, \mathbb{HP}^{d-1})$ is justified only when (i) we find a numerical solution of the conditions of Proposition 4.1 to which Theorem 3.1 applies, and (ii) the action of the symmetry group on our simplex has finite (zero-dimensional) stabilizer. Regarding (ii), we have checked this rigorously in all the cases in part (a) of Tables 4–7 (see Section 7.3). In Table 8, which deals with $\mathbb{OP}^2$, only 5–point simplices fail to satisfy condition (ii). In that case there is a 3–dimensional stabilizer. We accounted for this in Table 8.

Remark 4.4 By similar calculations based on the real and complex analogues of Proposition 4.1,

$$r(N, \mathbb{RP}^{d-1}) = dN - \frac{N(N-1)}{2} - d^2 + 1 \quad \text{and}$$
$$r(N, \mathbb{CP}^{d-1}) = (2d-1)N - \frac{N(N-1)}{2} - 2d^2 + 2.$$

Neither quantity is ever positive when $d > 2$, which explains why our methods do not apply to real and complex projective spaces: the system of equations cannot be nonsingular for any tight simplex whose stabilizer is zero-dimensional.

When we attempt to apply Proposition 4.1, there are three possible outcomes:

(a) we find an approximate numerical solution with surjective Jacobian, in which case we can prove existence using Theorem 3.1,

(b) we find an approximate numerical solution, but the Jacobian at that point is not surjective, or

(c) we cannot even find an approximate numerical solution to the system, in which case we conjecture that there exists no tight simplex.

In a few cases we encountered a fourth possibility:

(d) we find what appears to be an approximate solution but we are unable to converge to greater precision.

When this situation arose we tried both Newton's method and gradient descent for energy minimization (see Section 7.2), but we were unable to improve the error in the constraints beyond 10^{-5} (as compared to a numerical error of about 10^{-15} for cases (a) and (b)). In these cases we make no conjecture as to existence or nonexistence of solutions.

Tables 4, 5, 6 and 7 list our results for $d = 3$, $d = 4$, $d = 5$ and $d = 6$, respectively. Each table lists all values of N from $d + 2$ to the upper bound $2d^2 - d$ from Proposition 2.2. There is no intrinsic problem with extending to larger dimensions, although the calculations become increasingly time-consuming.

Theorem 4.5 *For the values of (N, d) listed in part* (a) *of Tables 4 through 7, there exist tight N–point simplices in $\mathbb{HP}^{d-1}$.*

In fact, near the points found by our computer program and exhibited in the auxiliary files, the moduli space of simplices has dimension exactly $r(N, \mathbb{HP}^{d-1})$. In the case of a singular Jacobian (part (b) of the tables) we report the *rank deficiency* ($\dim W - \operatorname{rank} Df(x_*)$ in the terminology of Theorem 3.1).

In $\mathbb{HP}^4$, as shown in Table 6, we first observe a gap between the tight simplices of sizes d and $d+1$ that always exist in $\mathbb{HP}^{d-1}$ and the range of simplices for which our method proves existence. The gap is real: there exists no 7–point tight simplex in $\mathbb{HP}^4$, because of Corollary 2.13. Similarly, there exists no 8–point tight simplex in $\mathbb{HP}^5$.

(a)		(b)		(c)
N	$r(N, \mathbb{HP}^2)$	N	rank deficiency	N
5	0	12	2	14
6	4	13	2	
7	7	15	14	
8	9			
9	10			
10	10			
11	9			

Table 4: Cases in $\mathbb{HP}^2$: (a) proven existence of tight simplices; (b) singular Jacobian; (c) conjectured nonexistence.

(a)				(c)
N	$r(N, \mathbb{HP}^3)$	N	$r(N, \mathbb{HP}^3)$	N
6	0	14	28	22–28
7	7	15	27	
8	13	16	25	
9	18	17	22	
10	22	18	18	
11	25	19	13	
12	27	20	7	
13	28	21	0	

Table 5: Cases in $\mathbb{HP}^3$: (a) proven existence of tight simplices; (c) conjectured nonexistence.

4.2 12– and 13–point simplices

The cases of 12– and 13–point simplices are somewhat special: the system of constraints specified by Proposition 4.1 has a rank deficiency. To prove existence of solutions using Theorem 3.1, a different approach is needed.

We take as our starting point the following observation: not only do tight 12–point simplices exist (numerically), but actually 12–point cyclic-symmetric simplices exist (again, numerically). By this we mean a simplex such that, if $(x, y, z) \in \mathbb{H}^3$ is a point in it, then so are (y, z, x) and (z, x, y), and these are three distinct points in $\mathbb{HP}^2$.

We would like to adapt Proposition 4.1 to find simplices with cyclic symmetry. Imposing this symmetry reduces the number of degrees of freedom we have, but it also reduces

(a)						(c)	(d)
N	$r(N,\mathbb{HP}^4)$	N	$r(N,\mathbb{HP}^4)$	N	$r(N,\mathbb{HP}^4)$	N	N
8	9	15	51	22	44	7	28
9	18	16	53	23	39	29–45	
10	26	17	54	24	33		
11	33	18	54	25	26		
12	39	19	53	26	18		
13	44	20	51	27	9		
14	48	21	48				

Table 6: Cases in $\mathbb{HP}^4$: (a) proven existence of tight simplices; (c) conjectured nonexistence (proven for $N=7$); (d) ambiguous numerical results.

(a)						(c)	(d)
N	$r(N,\mathbb{HP}^5)$	N	$r(N,\mathbb{HP}^5)$	N	$r(N,\mathbb{HP}^5)$	N	N
9	10	18	82	27	73	8	35
10	22	19	85	28	67	36–66	
11	33	20	87	29	60		
12	43	21	88	30	52		
13	52	22	88	31	43		
14	60	23	87	32	33		
15	67	24	85	33	22		
16	73	25	82	34	10		
17	78	26	78				

Table 7: Cases in $\mathbb{HP}^5$: (a) proven existence of tight simplices; (c) conjectured nonexistence (proven for $N=8$); (d) ambiguous numerical results.

the number of conditions we need to check. Fortunately, we end up with a set of constraints that has a surjective Jacobian at a tight simplex.

For convenience we will state the result only for $d=3$, but it naturally generalizes to any dimension (along the lines of Proposition 6.5).

Proposition 4.6 *Let σ be the cyclic-shift automorphism $\sigma(a,b,c)=(b,c,a)$. Suppose $x_1,\dots,x_{3m}\in\mathbb{H}^3$ and $w_1,\dots,w_{3m}\in\mathbb{R}$ satisfy the following conditions:*

(a) $x_{m+i}=\sigma(x_i)$ *for* $i=1,\dots,2m$,

(b) $w_{m+i}=w_i$ *for* $i=1,\dots,2m$,

(c) $|x_i|^2 = 1$ *for* $i = 1, \dots, m$,

(d) *the squared inner products* $|\langle x_i, x_j\rangle|^2$, *for* $i = 1, \dots, m$ *and the following values of* j, *are all equal:* (i) $j = i + m$, (ii) $i < j \le m$, (iii) $i + m < j \le 2m$, (iv) $i + 2m < j \le 3m$, *and*

(e) *the matrix* $\sum_{i=1}^{3m} w_i x_i x_i^\dagger$ *has* $(1,1)$ *entry equal to* 1 *and vanishing* $(1,2)$ *entry.*

Then $w_1 = \dots = w_{3m} = 1/m$ *and* $\{x_1, \dots, x_{3m}\}$ *is a tight simplex in* $\mathbb{HP}^2$.

Proof By repeated applications of $\langle x_i, x_j\rangle = \langle \sigma(x_i), \sigma(x_j)\rangle$, it easily follows that $\{x_1, \dots, x_{3m}\}$ is a simplex.

Having shown that, now consider the matrix $M = \sum_{i=1}^{3m} w_i x_i x_i^\dagger$. Rewriting M as $\sum_{i=1}^{m} w_i (x_i x_i^\dagger + \sigma(x_i)\sigma(x_i)^\dagger + \sigma^2(x_i)\sigma^2(x_i)^\dagger)$, we see that M is cyclic-symmetric; in other words, it is invariant under conjugation by the permutation σ. Of course M is also Hermitian. Combining these two properties, it must be of the form

$$M = \begin{pmatrix} r & s & \overline{s} \\ \overline{s} & r & s \\ s & \overline{s} & r \end{pmatrix}$$

for some $r \in \mathbb{R}$ and $s \in \mathbb{H}$. The last condition in the proposition statement forces $r = 1$ and $s = 0$, so in fact $M = I_3$.

Therefore, $\{x_1, \dots, x_{3m}\}$ is a simplex with $\sum_{i=1}^{3m} w_i x_i x_i^\dagger = I_3$, and we complete the proof by applying Proposition 4.1. □

Applying the constraints in the above proposition with $m = 4$, we get a surjective Jacobian in Theorem 3.1, which proves the following result.

Theorem 4.7 *There is a tight simplex of* 12 *points in* $\mathbb{HP}^2$*. In fact, there is such a tight simplex with cyclic symmetry.*

Experimentally it appears that tight simplices with cyclic symmetry exist in other cases, such as 6– and 9–point simplices in $\mathbb{HP}^2$. In those cases we do not need to use the symmetry to establish the existence of tight simplices, though.

For 13–point simplices, we wish to follow a similar approach to bypass the rank-deficiency issue, but we must allow fixed points of the cyclic shift. In fact, there are cyclic-symmetric 13–point tight simplices consisting of 12 points with cyclic symmetry as above (in other words, four equivalence classes under the cyclic-shift operator) plus one extra point which is invariant under the cyclic-shift operator.

Proposition 4.8 *Let σ be the cyclic-shift automorphism $\sigma(a,b,c)=(b,c,a)$. Suppose $x_1,\dots,x_{3m}\in\mathbb{H}^3$ satisfy the following conditions:*

(a) $x_{m+i}=\sigma(x_i)$ *for* $i=1,\dots,2m$,

(b) $|x_i|^2=1$ *for* $i=1,\dots,m$,

(c) *the squared inner products* $|\langle x_i,x_j\rangle|^2$, *for* $i=1,\dots,m$ *and the following values of* j, *are all equal:* (i) $j=i+m$, (ii) $i<j\le m$, (iii) $i+m<j\le 2m$, (iv) $i+2m<j\le 3m$, *and*

(d) *the* $(1,2)$ *entry of the matrix* $\sum_{i=1}^{3m} x_i x_i^\dagger$ *has real part* $\frac{1}{6}$ *and magnitude* $\frac{1}{3}$.

Then there is a unique point $x_{3m+1}\in\mathbb{HP}^2$ such that $\{x_1,\dots,x_{3m},x_{3m+1}\}$ is a tight simplex, and that point satisfies $\sigma(x_{3m+1})=x_{3m+1}$.

Proof A tight $(3m+1)$–point simplex $\{x_1,\dots,x_{3m+1}\}$ must satisfy

$$\sum_{i=1}^{3m+1} x_i x_i^\dagger = \frac{3m+1}{3} I_3.$$

Thus the matrix $x_{3m+1}x_{3m+1}^\dagger$ is determined by the other data; since a point in projective space is determined by its projection matrix, this proves uniqueness. It also proves that if such a point x_{3m+1} exists, then it must satisfy $\sigma(x_{3m+1})=x_{3m+1}$ up to scalar multiplication (by a cube root of unity in $\mathbb{H}$); this is because otherwise

$$\sigma(\{x_1,\dots,x_{3m},x_{3m+1}\})=\{x_1,\dots,x_{3m},\sigma(x_{3m+1})\}$$

would be a distinct tight simplex.

Define $M=\sum_{i=1}^{3m} x_i x_i^\dagger$. This matrix is Hermitian and cyclic-symmetric, so as in the proof of Proposition 4.6 it is of the form

$$M=\begin{pmatrix} r & s & \overline{s}\\ \overline{s} & r & s\\ s & \overline{s} & r\end{pmatrix}$$

for some $r\in\mathbb{R}$ and $s\in\mathbb{H}$. Each projection $x_i x_i^\dagger$ has trace 1, so $\operatorname{Tr} M=3m$ and thus $r=m$. Let

$$\begin{aligned}\Pi &:= \frac{3m+1}{3} I_3 - M\\ &= \begin{pmatrix} \frac{1}{3} & -s & -\overline{s}\\ -\overline{s} & \frac{1}{3} & -s\\ -s & -\overline{s} & \frac{1}{3}\end{pmatrix}.\end{aligned}$$

Being Hermitian and of trace 1, Π is a projection matrix of rank 1 if and only if $3s^2 = -\overline{s}$, as one can see by solving $\Pi^2 = \Pi$. The last hypothesis in the proposition statement implies that $-3s$ is a cube root of unity in $\mathbb{H}$, from which we see that this condition is satisfied.

Let $x_{3m+1} \in \mathbb{HP}^2$ be the point satisfying $\Pi = x_{3m+1}x_{3m+1}^\dagger$. We know $\{x_1, \dots, x_{3m}\}$ is a regular simplex, as in Proposition 4.6. For $i = 1, \dots, 3m$ define $\Pi_i = x_i x_i^\dagger$, and let α be the common inner product $\langle \Pi_i, \Pi_j \rangle$ for $i, j \le 3m$ with $i \ne j$. By the definition of Π,

$$\Pi + \sum_{i=1}^{3m} \Pi_i = \frac{3m+1}{3} I_3. \tag{4-2}$$

Since $\langle \Pi_i, \Pi_j \rangle = \alpha$ for $i \ne j$ and $\langle \Pi_i, \Pi_i \rangle = 1$, the symmetry of (4-2) implies that the inner products $\langle \Pi, \Pi_i \rangle$ are all equal; call their common value β. Taking the inner product of (4-2) with Π and Π_i yields

$$1 + 3m\beta = (3m+1)/3 \quad \text{and} \quad \beta + (3m-1)\alpha + 1 = (3m+1)/3,$$

respectively. Subtracting shows that $\alpha = \beta$, so $\{x_1, \dots, x_{3m+1}\}$ is a simplex, and it is tight by (4-2). □

We get a surjective Jacobian when we apply the conditions of the above proposition in Theorem 3.1 with $m = 4$, proving the following result.

Theorem 4.9 *There is a tight simplex of* 13 *points in* $\mathbb{HP}^2$*. In fact, there is such a tight simplex with cyclic symmetry.*

Theorems 4.7 and 4.9 establish the existence of tight simplices, and their proof could also provide the dimension of the space of tight simplices with cyclic symmetry. They cannot, though, tell us the dimension of the full space of tight simplices.

If Proposition 4.1 had applied then we would have concluded that in some neighborhood, the space of tight simplices of 12 (resp. 13) points in $\mathbb{HP}^2$ has dimension 7 (resp. 4). The observed rank deficiency of two has several possible explanations, including the following: it might mean that two of the constraints are redundant, so that the space of tight simplices is two dimensions larger than predicted; it might mean that the constraints become degenerate at the solutions, but the space of tight simplices is still a manifold; or it might mean that the space of tight simplices is not even locally a manifold. Based on numerical evidence (see Section 7.5), we conjecture that the first possibility holds.

Conjecture 4.10 *There exists a 12–point (resp. 13–point) tight simplex in $\mathbb{HP}^2$ such that, in a neighborhood thereof, the space of tight simplices has dimension 9 (resp. 6).*

4.3 15–point simplices

The case of 15 points in $\mathbb{HP}^2$ is special for a few reasons. First, it may be the only case in quaternionic projective spaces where the cardinality upper bound in Proposition 2.2 is achieved (beyond $\mathbb{HP}^1$, which is S^4 and clearly contains a 6–point simplex). Also, in comparison with the other cases in Table 4, this case has especially large rank deficiency. This suggests that the moduli space of simplices is of a larger dimension than $r(15, \mathbb{HP}^2)$. That turns out to be correct, as we now show.

Proposition 4.11 *Suppose $x_1, \dots, x_{15} \in \mathbb{H}^3$ satisfy*

$$\langle \Gamma_i, \Gamma_j \rangle = -\tfrac{1}{21} \quad \text{for } i \neq j,$$

where

$$\Gamma_i := x_i x_i^\dagger - \tfrac{1}{3}|x_i|^2 I_3.$$

Suppose additionally that $|x_i|^4 \in [1 - 10^{-6}, 1 + 10^{-6}]$ for each i. Then $|x_i| = 1$ and $\{x_1, \dots, x_{15}\}$ is a tight simplex in $\mathbb{HP}^2$.

We do not think the assumption $|x_i|^4 \in [1 - 10^{-6}, 1 + 10^{-6}]$ is necessary for the proposition to hold, but it is easy to verify in our applications and lets us prove the result with local calculations. This proof and that of Proposition 5.8 will be based on two technical lemmas (Lemmas 4.14 and 4.15), which we defer until the end of the section. It would be straightforward to replace them in our applications with bounds computed using interval arithmetic (see Section 7.2), but they are simple enough to prove by hand, so we do so below.

Proof For each i write $|x_i|^4 = 1 + \delta_i$, and let $\delta = \max_i |\delta_i|$. It suffices to show $\delta = 0$, because $\{x_1, \dots, x_{15}\}$ is then a tight simplex. Specifically, define $\eta_i = (1 + \delta_i)^{-1/2}$ and let $\Pi_i = x_i x_i^\dagger / |x_i|^2 = \eta_i x_i x_i^\dagger$ denote the projection matrix associated to x_i. Then

$$\langle \Pi_i, \Pi_j \rangle = \eta_i \eta_j \langle \Gamma_i, \Gamma_j \rangle + \tfrac{1}{3} = \begin{cases} 1 & \text{if } i = j, \\ -\eta_i \eta_j / 21 + \frac{1}{3} & \text{if } i \neq j. \end{cases}$$

If $\eta_i = 1$ for all i, then these inner products agree with the desired value $2/7$ in a tight simplex of 15 points.

Our strategy is to show that nonnegativity of the second zonal harmonic sum forces $\delta = 0$, given a rank condition coming from the fact that 15 equals the dimension of the space of Hermitian matrices.

Recall that the zonal harmonics on $\mathbb{HP}^{d-1}$ are given by Jacobi polynomials

$$P_k^{(2d-3,1)}(2t-1).$$

Specifically, the functions

$$K_k(x,y) = P_k^{(2d-3,1)}(2|\langle x,y\rangle|^2-1)$$

are positive-definite kernels on $\mathbb{HP}^{d-1}$. Let Σ_k be the sum of the kernel $K_k(x,y)$ over the projective code determined by $\{x_1,\dots,x_{15}\}$. Then positive definiteness implies $\Sigma_k \geq 0$.

We will require only Σ_2. As $P_2(3,1)(2t-1) = 28t^2-21t+3$, we can write Σ_2 in terms of the moments $\sum_{i,j=1}^{15}\langle \Pi_i,\Pi_j\rangle^k$ with $k\leq 2$. If $\delta=0$, then $\Sigma_2=0$, and we wish to compute it to second order in $\delta_1,\dots,\delta_{15}$ in terms of the moments $m_1 := \sum_i \delta_i$ and $m_2 := \sum_i \delta_i^2$. Applying Lemma 4.14 with $P_{i,j}=\langle \Pi_i,\Pi_j\rangle$, we find that

$$\left|\Sigma_2 - \left(-\tfrac{10}{3}m_1 + \tfrac{23}{252}m_1^2 + \tfrac{719}{252}m_2\right)\right| \leq 8295\cdot\delta^3. \tag{4-3}$$

If we could approximate Σ_2 sufficiently well by a negative-definite quadratic form in $\delta_1,\dots,\delta_{15}$, then $\Sigma_2\geq 0$ would imply $\delta=0$. However, the approximation in (4-3) is not negative-definite. To make it so, we must add correction terms based on additional constraints satisfied by the perturbations δ_i.

These additional constraints come from a singular Gram matrix. We have $\langle\Gamma_i,\Gamma_i\rangle = \frac{2}{3}(1+\delta_i)$, and the Gram matrix of the elements $\sqrt{2/3}\,\Gamma_i$ is

$$G = \begin{pmatrix} 1+\delta_1 & & -\frac{1}{14} \\ & \ddots & \\ -\frac{1}{14} & & 1+\delta_N \end{pmatrix}.$$

Each of $\Gamma_1,\dots,\Gamma_{15}$ is a traceless Hermitian matrix, so they must be linearly dependent, because the space of such matrices has dimension 14. Thus, the Gram matrix G must be singular. Let $D := 14^{14}\det(G)/15^{12}$ be its determinant, normalized as in Lemma 4.15. Of course $D=0$, but we know from Lemma 4.15 that

$$|D-15m_1-14(m_1^2-m_2)| \leq 50625\cdot\delta^3 \quad\text{and}\quad |D^2-225m_1^2|\leq 4556250\cdot\delta^3.$$

Because D (and so D^2) must vanish and Σ_2 must be nonnegative,

$$\Sigma_2' := 4200D - 269D^2 + 18900\Sigma_2$$

must be nonnegative as well. However, from the above inequalities, we have

$$|\Sigma_2' + 4875m_2| \leq 16\cdot 10^8\cdot\delta^3.$$

We have $-4875 m_2 \le -4875 \cdot \delta^2$, and the assumption $\delta \le 10^{-6}$ implies that

$$16 \cdot 10^8 \cdot \delta^3 \le 4875 \cdot \delta^2.$$

It follows that $\Sigma_2' \le 0$, with equality if and only if $\delta = 0$. Because Σ_2' is nonnegative, we conclude that indeed equality must hold, as desired. □

Using this system of constraints, we do get a nonsingular Jacobian matrix and hence we can apply Theorem 3.1. This yields a 75–dimensional solution space; after subtracting overcounting and symmetries, we arrive at the following.

Theorem 4.12 *There is a tight simplex of* 15 *points in* $\mathbb{HP}^2$*. In fact, locally there is a* 9*–dimensional space of such simplices.*[5]

Theorem 4.12 establishes the existence of a tight 2–design in $\mathbb{HP}^2$. The common inner product in this simplex is $\frac{2}{7}$, contrary to a theorem of Bannai and Hoggar asserting that the inner products in tight designs are always reciprocals of integers [12, Corollary 1.7(b)]. The case of 2–designs is not addressed in their proof, and Bannai has informed us that this was an oversight in the theorem statement. See also [58] for another correction (the icosahedron is a tight 5–design in $\mathbb{CP}^1$ with irrational inner products).

It would be interesting to determine whether using the points of a 15–point simplex as vertices could lead to a minimal triangulation of $\mathbb{HP}^2$ (see [21]), as well as whether the same is true for a 27–point simplex in $\mathbb{OP}^2$.

Tight 2–designs in $\mathbb{HP}^{d-1}$ are quaternionic analogues of SIC-POVMs [67]. Because SIC-POVMs seem to exist in $\mathbb{CP}^{d-1}$ for every d, it is natural to speculate that tight quaternionic 2–designs should be even more abundant, but we have not found any examples with $d > 3$.

So far, we have shown that there are tight simplices in $\mathbb{HP}^2$ of every size up to 15 except for 14.

Conjecture 4.13 *There does not exist a tight simplex of* 14 *points in* $\mathbb{HP}^2$*.*

Similarly, we will see in Section 5 that there are tight simplices in $\mathbb{OP}^2$ of every size up to 27 except for 26. In $\mathbb{RP}^2$ every size up to 6 except for 5 occurs, while in $\mathbb{CP}^2$ we see every size up to 9 except for 5 and 8. It seems unlikely to be a coincidence that the second largest possible size is always missing in projective planes, but we do not have a proof beyond $\mathbb{RP}^2$. (As explained after Lemma 2.9, linear programming

[5] As opposed to the absurd -5 predicted by $r(15, \mathbb{HP}^2)$.

bounds suffice to disprove the existence of tight 5–point simplices in $\mathbb{RP}^2$. However, they do not rule out the analogous cases in $\mathbb{CP}^2$, $\mathbb{HP}^2$ or $\mathbb{OP}^2$.)

In the remainder of this section, we state and prove the deferred lemmas from the proof of Proposition 4.11.

Lemma 4.14 *Given $d \geq 2$, $N > 1$, and $\delta_1, \dots, \delta_N$ with $\delta := \max_i |\delta_i| \leq \frac{1}{4}$, set $\eta_i = (1+\delta_i)^{-1/2}$, $\lambda = -(d-1)/(d(N-1))$, $m_1 = \sum_i \delta_i$, $m_2 = \sum_i \delta_i^2$, and*

$$P_{i,j} = \begin{cases} 1 & \text{if } i = j, \\ \eta_i \eta_j \lambda + 1/d & \text{if } i \neq j. \end{cases}$$

Let

$$\begin{aligned}
T_0 &= N^2, \\
T_1 &= \frac{N^2}{d} + \frac{d-1}{d} m_1 + \lambda\Big(\frac{3N}{4} - 1\Big) m_2 + \frac{\lambda}{4} m_1^2, \\
T_2 &= \frac{N^2(N+d^2-2d)}{d^2(N-1)} - \frac{2(N-d)\lambda}{d} m_1 \\
&\qquad\qquad + \lambda\Big(\lambda + \frac{1}{2d}\Big) m_1^2 - \frac{\lambda}{d}\Big((2+\lambda)d - \frac{3N}{2}\Big) m_2.
\end{aligned}$$

Then the moments $S_k := \sum_{i,j=1}^N P_{i,j}^k$ satisfy the bounds

$$S_0 = T_0, \quad |S_1 - T_1| \leq 5N\delta^3 \quad \text{and} \quad |S_2 - T_2| \leq 16N\delta^3.$$

Proof It is clear that $S_0 = N^2$. For S_1 and S_2, we begin by explicitly computing

$$\begin{aligned}
S_1 &= \lambda\Big(\sum_{i=1}^N \eta_i\Big)^2 - \lambda\Big(\sum_{i=1}^N \eta_i^2\Big) + \frac{N^2-N+Nd}{d}, \\
S_2 &= \lambda^2\Big(\sum_{i=1}^N \eta_i^2\Big)^2 - \lambda^2\Big(\sum_{i=1}^N \eta_i^4\Big) + \frac{2\lambda}{d}\Big(\sum_{i=1}^N \eta_i\Big)^2 - \frac{2\lambda}{d}\Big(\sum_{i=1}^N \eta_i^2\Big) \\
&\qquad + \frac{N^2+Nd^2-N}{d^2}.
\end{aligned}$$

Now, using $\eta_i = (1+\delta_i)^{-1/2}$ and $\delta \leq \frac{1}{4}$, Taylor's theorem with the Lagrange form of the remainder yields the estimates

$$\Big|\eta_i^a - \big(1 - \tfrac{1}{2}a\delta_i + \tfrac{1}{4}a(a+2)\cdot\tfrac{1}{2}\delta_i^2\big)\Big| \leq \tfrac{4}{81}\big(\tfrac{4}{3}\big)^{a/2} a(a+2)(a+4)\cdot\delta^3$$

for all $a > 0$. Taking $a = 1, 2, 4$ we get, respectively, the bounds

$$\left|\sum_{i=1}^{N} \eta_i - \left(N - \tfrac{1}{2}m_1 + \tfrac{3}{8}m_2\right)\right| \le N\delta^3,$$
$$\left|\sum_{i=1}^{N} \eta_i^2 - (N - m_1 + m_2)\right| \le 4N\delta^3,$$
$$\left|\sum_{i=1}^{N} \eta_i^4 - (N - 2m_1 + 3m_2)\right| \le 17N\delta^3.$$

We also have the simple bounds $|m_i| \le N\delta^i$. Using these, we find

$$\begin{aligned}
&\left|\left(\sum_{i=1}^{N} \eta_i\right)^2 - \left(N^2 - Nm_1 + \tfrac{3}{4}Nm_2 + \tfrac{1}{4}m_1^2\right)\right| \\
&\qquad\le \left|\left(\sum_{i=1}^{N} \eta_i\right)^2 - \left(N - \tfrac{1}{2}m_1 + \tfrac{3}{8}m_2\right)^2\right| + \left|\tfrac{3}{8}m_1m_2 - \tfrac{9}{64}m_2^2\right| \\
&\qquad\le N\delta^3 \cdot \left|\sum_{i=1}^{N} \eta_i + N - \tfrac{1}{2}m_1 + \tfrac{3}{8}m_2\right| + N^2\left(\tfrac{3}{8}\delta^3 + \tfrac{9}{64}\delta^4\right) \\
&\qquad\le N\delta^3\left(2\left|N - \tfrac{1}{2}m_1 + \tfrac{3}{8}m_2\right| + N\delta^3\right) + N^2\left(\tfrac{3}{8}\delta^3 + \tfrac{9}{64}\delta^4\right) \\
&\qquad\le N\delta^3\left(2N\left(1 + \tfrac{1}{2}\delta + \tfrac{3}{8}\delta^2\right) + N\delta^3\right) + N^2\left(\tfrac{3}{8}\delta^3 + \tfrac{9}{64}\delta^4\right) \\
&\qquad\le 3N^2\delta^3.
\end{aligned}$$

We similarly compute

$$\left|\left(\sum_{i=1}^{N} \eta_i^2\right)^2 - (N^2 - 2Nm_1 + 2Nm_2 + m_1^2)\right| \le 13N^2\delta^3.$$

Combining all of these estimates with $d \ge 2$, $N \ge 2$ and $|\lambda| \le 1/N$ leads to bounds of $(3N+4)\delta^3$ and $(3N+17+17/N)\delta^3$ for $|S_1 - T_1|$ and $|S_2 - T_2|$ respectively. We have rounded them up to pleasant multiples of N in the lemma statement. □

Lemma 4.15 *Suppose $N > 3$, and let*

$$D = \frac{(N-1)^{N-1}}{N^{N-3}} \det \begin{pmatrix} 1+\delta_1 & & -\frac{1}{N-1} \\ & \ddots & \\ -\frac{1}{N-1} & & 1+\delta_N \end{pmatrix},$$

where every off-diagonal entry in the above matrix equals $-1/(N-1)$. Set $\delta = \max_i |\delta_i|$, $m_1 = \sum_i \delta_i$ and $m_2 = \sum_i \delta_i^2$. If $\delta \le 1/(2N)$, then

$$|D - Nm_1 - (N-1)(m_1^2 - m_2)| \le N^4\delta^3 \quad \text{and} \quad |D^2 - N^2 m_1^2| \le 6N^5\delta^3.$$

Proof Let G_r be the $r \times r$ matrix with diagonal entries 1 and off-diagonal entries β. It is easy to show[6] that

$$D_r := \det(G_r) = (1 + (r-1)\beta)(1-\beta)^{r-1}.$$

Setting $\beta = -1/(N-1)$, we have

$$D_r = \frac{(N-r)N^{r-1}}{(N-1)^r}.$$

Using this, for

$$G = \begin{pmatrix} 1+\delta_1 & & -\frac{1}{N-1} \\ & \ddots & \\ -\frac{1}{N-1} & & 1+\delta_N \end{pmatrix}$$

we find that

$$\begin{aligned} \det(G) &= D_N + \Big(\sum_i \delta_i\Big) D_{N-1} + \Big(\sum_{i<j} \delta_i\delta_j\Big) D_{N-2} + \cdots + \prod_i \delta_i \\ &= 0 + \Big(\sum_i \delta_i\Big) \frac{N^{N-2}}{(N-1)^{N-1}} + \Big(\sum_{i<j} \delta_i\delta_j\Big) \frac{2N^{N-3}}{(N-1)^{N-2}} + \cdots + \prod_i \delta_i. \end{aligned}$$

In terms of the moments $m_1 = \sum_i \delta_i$ and $m_2 = \sum_i \delta_i^2$, the rescaled determinant $D = (N-1)^{N-1}\det(G)/N^{N-3}$ satisfies

$$|D - Nm_1 - (N-1)(m_1^2 - m_2)| \le \sum_{k \ge 3} \binom{N}{k} \delta^k N^{2-k}(N-1)^{k-1}k.$$

The $k = 3$ term on the right is $(N-1)^3(N-2)\delta^3/2 \le N^4\delta^3/2$. Because $\delta \le 1/(2N)$, each subsequent term diminishes by a factor of at least $\frac{1}{2}$. Thus, summing the geometric series, we have

$$|D - Nm_1 - (N-1)(m_1^2 - m_2)| \le N^4\delta^3.$$

[6] See the footnote in the proof of Proposition 2.2.

Note that the trivial bounds $|m_1| \le N\delta$ and $m_2 \le N\delta^2$ imply

$$\begin{aligned} |Nm_1 + (N-1)(m_1^2 - m_2)| &\le N^2\delta + (N-1)(N^2\delta^2 + N\delta^2) \\ &= N^2\delta + N(N^2-1)\delta^2 \\ &\le N^2\delta + N^3\delta^2 \le 2N^2\delta, \end{aligned}$$

and therefore $|D| \le 2N^2\delta + N^4\delta^3 \le 3N^2\delta$. Now, to control D^2, we write

$$\begin{aligned} |D^2 - (Nm_1 + (N-1)(m_1^2 - m_2))^2| &\le N^4\delta^3 |D + Nm_1 + (N-1)(m_1^2 - m_2)| \\ &\le N^4\delta^3(|D| + |Nm_1 + (N-1)(m_1^2 - m_2)|) \\ &\le N^4\delta^3(5N^2\delta) = 5N^6\delta^4. \end{aligned}$$

Furthermore,

$$\begin{aligned} &|N^2m_1^2 - (Nm_1 + (N-1)(m_1^2 - m_2))^2| \\ &\qquad \le 2N(N-1)|m_1|(m_1^2 + m_2) + (N-1)^2(m_1^2 + m_2)^2 \\ &\qquad \le 2N(N-1)N\delta(N^2\delta^2 + N\delta^2) + (N-1)^2(N^2\delta^2 + N\delta^2)^2 \\ &\qquad = 2N^3(N^2-1)\delta^3 + N^2(N^2-1)^2\delta^4 \le 3N^5\delta^3. \end{aligned}$$

Combining these two bounds with the triangle inequality and using $N\delta \le \frac{1}{2}$, we obtain the asserted bound for $|D^2 - N^2m_1^2|$. □

5 Simplices in $\mathbb{OP}^2$

The study of simplices in $\mathbb{OP}^2$ unfolds much like that in $\mathbb{HP}^2$; we get essentially the same results as long as we take care to work in an affine chart. In particular, we can handle the generic case, 24– and 25–point simplices, and 27–point simplices using adaptations of Propositions 4.1, 4.6 and 4.8, and 4.11, respectively.

5.1 Generic case

Proposition 5.1 *For $i = 1, \dots, N$, suppose $x_i = (a_i, b_i, c_i) \in \mathbb{R}_+ \times \mathbb{O}^2$ and $w_i \in \mathbb{R}$ satisfy*

(a) $|a_i|^2 + |b_i|^2 + |c_i|^2 = 1$ *for* $i = 1, \dots, N$,

(b) $\rho(x_i, x_j)^2 = \rho(x_{i'}, x_{j'})^2$ *for* $1 \le i < j \le N$ *and* $1 \le i' < j' \le N$, *and*

(c) *the matrix equation*

$$\sum_{i=1}^{N} w_i \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix} \begin{pmatrix} \overline{a}_i & \overline{b}_i & \overline{c}_i \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then $w_1 = \cdots = w_N = 3/N$ *and* $\{x_1, \dots, x_N\}$ *is a tight simplex.*

We omit the proof of Proposition 5.1 as it is nearly identical to that of Proposition 4.1.

We can attempt to apply Proposition 5.1 with Theorem 3.1 just as we did for simplices in quaternionic projective spaces. There are

$$N + \left(\frac{N(N-1)}{2} - 1\right) + 27$$

real constraints in $18N$ real variables, so when the Jacobian is nonsingular we get a solution space of dimension $(N-1)(34-N)/2 - 9$. As before, we should deduct the dimension of the symmetry group. The symmetry group of $\mathbb{OP}^2$ is the exceptional Lie group F_4, which has dimension 52. Thus, our final expression for the expected local dimension of the moduli space of simplices is

$$r(N, \mathbb{OP}^2) := \frac{(N-1)(34-N)}{2} - 61.$$

Again, as with $r(N, \mathbb{HP}^{d-1})$, this formula only applies when, at our numerical solution, Theorem 3.1 applies to the conditions of Proposition 5.1 and the simplex has zero-dimensional stabilizer.

Theorem 5.2 *For the values of* N *listed in part (a) of Table 8, there exist tight* N*–point simplices in* $\mathbb{OP}^2$*.*

5.2 24– and 25–point simplices

The following proposition is proven similarly to Proposition 4.6.

Proposition 5.3 *Let* σ *be the cyclic-shift automorphism* $\sigma(a,b,c) = (b,c,a)$*. Suppose* $x_1, \dots, x_{3m} \in \mathbb{O}^3$ *and* $w_1, \dots, w_{3m} \in \mathbb{R}$ *satisfy the following conditions:*

- (a) $x_{m+i} = \sigma(x_i)$ *for* $i = 1, \dots, 2m$,
- (b) $w_{m+i} = w_i$ *for* $i = 1, \dots, 2m$,
- (c) $x_i \in \mathbb{R}_+ \times \mathbb{O}^2$ *and* $|x_i|^2 = 1$ *for* $i = 1, \dots, m$,
- (d) *the squared distances* $\rho(x_i, x_j)^2$*, for* $i = 1, \dots, m$ *and the following values of* j*, are all equal:* (i) $j = i + m$, (ii) $i < j \le m$, (iii) $i + m < j \le 2m$, (iv) $i + 2m < j \le 3m$, *and*
- (e) *the matrix* $\sum_{i=1}^{3m} w_i x_i x_i^\dagger$ *has* $(1,1)$ *entry equal to* 1 *and vanishing* $(1,2)$ *entry.*

Then $w_1 = \cdots = w_{3m} = 1/m$ *and* $\{x_1, \dots, x_{3m}\}$ *is a tight simplex.*

(a)						(b)		(c)
N	$r(N, \mathbb{OP}^2)$	N	$r(N, \mathbb{OP}^2)$	N	$r(N, \mathbb{OP}^2)$	N	rank deficiency	N
5	$0^\dagger$	12	60	19	74	24	2	26
6	9	13	65	20	72	25	2	
7	20	14	69	21	69	27	26	
8	30	15	72	22	65			
9	39	16	74	23	60			
10	47	17	75					
11	54	18	75					

Table 8: Cases in $\mathbb{OP}^2$: (a) proven existence of tight simplices; (b) singular Jacobian; (c) conjectured nonexistence.

†Actually $r(5, \mathbb{OP}^2)$ is not 0; rather, it equals -3. This is the only case in which the simplex we found has a positive-dimensional stabilizer. The stabilizer is 3–dimensional, so the actual dimension of the moduli space, which is what $r(5, \mathbb{OP}^2)$ is really intended to capture, is 0.

Using the conditions of Proposition 5.3 with $m = 8$ in Theorem 3.1 yields a surjective Jacobian, allowing us to prove the following theorem.

Theorem 5.4 *There is a tight simplex of* 24 *points in* $\mathbb{OP}^2$*. In fact, there is such a tight simplex with cyclic symmetry.*

Similarly, to prove the existence of tight simplices with 25 points, we use the following adaptation of Proposition 4.8.

Proposition 5.5 *Let* σ *be the cyclic-shift automorphism* $\sigma(a, b, c) = (b, c, a)$*. Suppose* $x_1, \dots, x_{3m} \in \mathbb{O}^3$ *satisfy the following conditions:*

(a) $x_{m+i} = \sigma(x_i)$ *for* $i = 1, \dots, 2m$,

(b) $x_i \in \mathbb{R}_+ \times \mathbb{O}^2$ *and* $|x_i|^2 = 1$ *for* $i = 1, \dots, m$,

(c) *the squared distances* $\rho(x_i, x_j)^2$*, for* $i = 1, \dots, m$ *and the following values of* j*, are all equal:* (i) $j = i + m$, (ii) $i < j \le m$, (iii) $i + m < j \le 2m$, (iv) $i + 2m < j \le 3m$*, and*

(d) *the* $(1, 2)$ *entry of the matrix* $\sum_{i=1}^{3m} x_i x_i^\dagger$ *has real part* $\frac{1}{6}$ *and magnitude* $\frac{1}{3}$.

Then there is a unique point $x_{3m+1} \in \mathbb{OP}^2$ *such that* $\{x_1, \dots, x_{3m}, x_{3m+1}\}$ *is a tight simplex, and that point satisfies* $\sigma(x_{3m+1}) = x_{3m+1}$.

Using the conditions above with $m = 8$ in Theorem 3.1 yields a surjective Jacobian.

Theorem 5.6 *There is a tight simplex of 25 points in $\mathbb{OP}^2$. In fact, there is such a tight simplex with cyclic symmetry.*

Continuing the correspondence with 12– and 13–point simplices in $\mathbb{HP}^2$, based on numerical evidence we conjecture the following.

Conjecture 5.7 *There exists a 24–point (resp. 25–point) tight simplex in $\mathbb{OP}^2$ such that in a neighborhood thereof, the space of tight simplices has dimension 56 (resp. 49).*

5.3 27–point simplices

Proposition 5.8 *Suppose $x_i = (a_i, b_i, c_i) \in \mathbb{R}_+ \times \mathbb{O}^2$ satisfy*

$$\langle \Gamma_i, \Gamma_j \rangle = -\tfrac{1}{39} \quad \text{for } i \neq j,$$

where

$$\Gamma_i := \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix} \begin{pmatrix} \overline{a}_i & \overline{b}_i & \overline{c}_i \end{pmatrix} - \tfrac{1}{3}\big(a_i^2 + |b_i|^2 + |c_i|^2\big) I_3.$$

Suppose additionally that $|x_i|^4 \in [1 - 10^{-7}, 1 + 10^{-7}]$ for each i. Then $|x_i| = 1$ and $\{x_1, \dots, x_{27}\}$ determines a tight simplex in $\mathbb{OP}^2$.

Proof We use the same proof technique as Proposition 4.11, with the only difference being the constants appearing in the proof.

As before, we write $|x_i|^4 = 1 + \delta_i$, and let $\delta = \max_i |\delta_i|$. Let G be the Gram matrix of $\sqrt{2/3}\,\Gamma_1, \dots \sqrt{2/3}\,\Gamma_{27}$. Then $\det(G) = 0$, and by Lemma 4.15 the normalized determinant $D := 26^{26} \det(G)/27^{24}$ satisfies

$$|D - 27m_1 - 26(m_1^2 - m_2)| \leq 531441 \cdot \delta^3 \quad \text{and} \quad |D^2 - 729m_1^2| \leq 86093442 \cdot \delta^3.$$

The second zonal harmonic on $\mathbb{OP}^2$ is given by the Jacobi polynomial

$$P_2^{(7,3)}(2t - 1) = 91t^2 - 65t + 10.$$

Let Σ_2 be the sum of the kernel $K_2(x, y) := P_2^{(7,3)}(2|\langle x, y\rangle|^2 - 1)$ over the projective code determined by $\{x_1, \dots, x_{27}\}$, so $\Sigma_2 \geq 0$. By Lemma 4.14,

$$\big|\Sigma_2 - \big(-6m_1 + \tfrac{41}{468}m_1^2 + \tfrac{2429}{468}m_2\big)\big| \leq 48087 \cdot \delta^3.$$

Because $D = 0$,

$$\Sigma_2' := 75816D - 2745D^2 + 341172\Sigma_2$$

must be nonnegative, but $|\Sigma_2' + 200475m_2| \leq 293024167110 \cdot \delta^3$. Since $m_2 \geq \delta^2$, when $\delta \leq 10^{-7}$ we have $\Sigma_2' \leq 0$ with equality only when $\delta = 0$. Thus, $\delta = 0$ and $\{x_1, \dots, x_{27}\}$ determines a tight simplex in $\mathbb{O}\mathbb{P}^2$. $\square$

Applying Theorem 3.1 with the conditions of the above proposition, we find a suitable point for which the Jacobian is surjective.

Theorem 5.9 *There is a tight simplex of* 27 *points in* $\mathbb{O}\mathbb{P}^2$*. In fact, locally there is a* 56*–dimensional space of such simplices.*

Theorem 5.9 establishes the existence of a tight 2–design in $\mathbb{O}\mathbb{P}^2$. Such designs were previously conjectured not to exist [43, page 251]. It is known [45] that tight t–designs in $\mathbb{O}\mathbb{P}^2$ can only exist for $t = 2$ and $t = 5$, and there is an explicit construction of a 819–point tight 5–design [27], so Theorem 5.9 completes the list of t for which tight t–designs exist in $\mathbb{O}\mathbb{P}^2$.

Conjecture 5.10 *There does not exist a tight simplex of* 26 *points in* $\mathbb{O}\mathbb{P}^2$*.*

See also the discussion after Conjecture 4.13.

6 Simplices in real Grassmannians

Our techniques also apply to show the existence of many simplices in Grassmannian spaces. The real Grassmannian $G(m, n)$ is the space of all m–dimensional subspaces of $\mathbb{R}^n$. It is a homogeneous space for the orthogonal group $O(n)$, isomorphic to $O(n)/(O(m) \times O(n-m))$, and it has dimension $m(n-m)$. These spaces generalize (real) projective space $\mathbb{R}\mathbb{P}^{n-1}$, which is the space of lines in $\mathbb{R}^n$. The spaces $G(m, n)$ and $G(n-m, n)$ can be identified by associating to each subspace its orthogonal complement, so in what follows we always assume $m \leq n/2$.

Though Grassmannians are generally not 2–point homogeneous spaces, there are still linear programming bounds [5; 6]. Here we will just consider the special case of the simplex bound.

When $m \leq n/2$, a pair of points in $G(m, n)$ is described by m parameters, namely the *principal angles* between the m–dimensional subspaces. Given two m–dimensional subspaces U and U', inductively define sequences of unit vectors $u_1, \dots, u_m \in U$

and $u'_1, \dots, u'_m \in U'$ so that $\langle u_i, u'_i \rangle$ is maximized subject to $\langle u_i, u_j \rangle = \langle u'_i, u'_j \rangle = 0$ for $j < i$. Then the principal angles are $\theta_i := \arccos\langle u_i, u'_i \rangle$.

The *chordal distance* on $G(m,n)$ is given by

$$d_c(U,U') = \sqrt{\sin^2\theta_1 + \cdots + \sin^2\theta_m}.$$

Unlike in projective space, the chordal metric on Grassmannians is generally not equivalent to the geodesic metric $\sqrt{\theta_1^2 + \cdots + \theta_m^2}$. See [31] for discussion of why the chordal metric is preferable.

A *generator matrix* for an element of $G(m,n)$ is an $m \times n$ matrix whose rows form an orthonormal basis of the subspace. Given a generator matrix X, the orthogonal projection onto the subspace is $X^t X$. Suppose X_1 and X_2 are generator matrices for the subspaces U_1 and U_2, and let $\Pi_i = X_i^t X_i$ (for $i = 1, 2$) be the orthogonal projection matrices. Then the singular values of the matrix $X_1 X_2^t$ are $\cos\theta_i$ for $1 \le i \le m$. It follows that

$$d_c(U_1,U_2)^2 = \tfrac{1}{2}\|\Pi_1 - \Pi_2\|_F^2 = m - \langle \Pi_1, \Pi_2 \rangle. \tag{6-1}$$

Let $\Pi^0 = \Pi - (m/n)I_n$ be the traceless part of the projection matrix. It can be thought of as a point in $\mathbb{R}^D$, where $D = m(m+1)/2 - 1$, if we view $\mathbb{R}^D$ as the space of trace-zero symmetric matrices. It is easily checked that $\|\Pi^0\|_F^2 = m(n-m)/n$. Therefore we obtain an isometric embedding $U \mapsto \Pi^0$ of $G(m,n)$ into the sphere of radius $\sqrt{m(n-m)/n}$ in $\mathbb{R}^D$ under the chordal metric. The simplex bound for spherical codes gives us the following result.

Proposition 6.1 (Conway, Hardin and Sloane [31]) *Every N–point simplex in $G(m,n)$ satisfies*

$$N \le \binom{m+1}{2},$$

and every code of N points has squared chordal distance at most

$$\frac{m(n-m)}{n} \cdot \frac{N}{N-1}.$$

This squared chordal distance is equivalent to having inner product

$$\frac{m(Nm-n)}{n(N-1)} \tag{6-2}$$

between orthogonal projection matrices.

Remark 6.2 The $m = 1$ case of Proposition 6.1 is the same as the $K = \mathbb{R}$ case of Proposition 2.2 (together with Proposition 2.4). Indeed, the proofs of these two results are essentially the same; they are just phrased in different language.

We say that a simplex in $G(m,n)$ is tight if its minimal chordal distance meets the upper bound above. Analogously to simplices in projective space, a Grassmannian simplex is tight if and only if it is a 1–design (a 2–design in the terminology of [7]), which holds if and only if the linear programming bound is sharp [5]. If the projection matrices of the simplex are $\Pi_1, \dots, \Pi_N$, then another equivalent condition for tightness is $\sum_{i=1}^N \Pi_i = (Nm/n)I_n$.

Conway, Hardin and Sloane [31] reported a number of putative tight simplices based on numerical evidence, but except for a few explicit constructions they did not present any techniques for rigorous existence proofs. (As in non-real projective spaces, it is not easy to reconstruct an exact Grassmannian simplex from a numerical approximation.) The cases with explicit constructions are listed in Table 9. By applying our methods, we can certify the existence of simplices for many of the cases previously identified but not settled.

(m,n)	N	Reference
$(2,4)$	2–6	[31, pages 145–146]
$(2,4)$	10	[31, page 147]
$(2,6)$	9	[31, page 154]
$(3,7)$	28	[31, page 152]
$(2,8)$	8	[31, page 154]
$(2,8)$	20	[22, page 135]
$(2,8)$	28	[31, page 154]

Table 9: Previously known tight simplices with explicit constructions in $G(m,n)$ for $n \le 8$.

Proposition 6.3 *Suppose that* $\{x_{i,j} \in \mathbb{R}^n\}_{i=1,\dots,N;\, j=1,\dots,m}$ *and* $w_1, \dots, w_N$ *satisfy the following conditions:*

(a) $|x_{i,j}| = 1$ *for all* i, j,

(b) *for all* i *and all* $j < j'$, $\langle x_{i,j}, x_{i,j'} \rangle = 0$,

(c) *the inner products* $\left\langle \sum_{j=1}^m x_{i,j} x_{i,j}^t, \sum_{j=1}^m x_{i',j} x_{i',j}^t \right\rangle$ *are equal for all distinct pairs* i, i', *and*

(d) $\sum_{i=1}^N w_i \left(\sum_{j=1}^m x_{i,j} x_{i,j}^t \right) = I_n$.

Then $w_1 = \cdots = w_N = n/(Nm)$ and the subspaces $\operatorname{span}\{x_{i,1}, \dots, x_{i,m}\}$ *form a tight simplex in* $G(m,n)$*.*

Proof For each i, define $\Pi_i = \sum_{j=1}^{m} x_{i,j} x_{i,j}^t$. Since $\{x_{i,1}, \dots, x_{i,m}\}$ is an orthonormal system, this is the projection matrix associated to the plane $\operatorname{span}\{x_{i,1}, \dots, x_{i,m}\}$. Using (6-1), the third condition guarantees that we have a simplex. Arguing as in the proof of Proposition 4.1, we deduce from the last condition that $w_i = n/(Nm)$ for each i. Thus $\sum_{i=1}^{N} \Pi_i = (Nm/n) I_n$; as noted above, this is equivalent to tightness. □

In many cases the system specified by Proposition 6.3 is nonsingular, allowing us to apply Theorem 3.1. This yields the following.

Theorem 6.4 *For the values of (N,m,n) listed in the "proven" column of Table 10, there exist tight N–point simplices in $G(m,n,\mathbb{R})$.*

In the context of Proposition 6.3, we have $Nmn + N$ real variables and

$$N \cdot \binom{m+1}{2} + \frac{N(N-1)}{2} - 1 + \binom{n+1}{2}$$

real constraints. Thus, when Theorem 3.1 applies, we locally get a solution space whose dimension is the difference of these counts. Because $O(m)$ acts on the different representations of each plane, we are overcounting the dimension by $N \cdot \binom{m}{2}$. Moreover, when the symmetry group $O(n)$ of $G(m,n)$ acts with finite stabilizer on the simplex, we should deduct $\binom{n}{2}$ from our final dimension count. Putting this all together, when these conditions are satisfied (as in Remark 4.3), we get a neighborhood in which the moduli space of simplices has dimension

$$r(N, G(m,n)) := Nmn - \frac{N(N-3)}{2} - Nm^2 - n^2 + 1. \tag{6-3}$$

As in projective spaces, we expect to find tight simplices in most cases for which $r(N, G(m,n)) > 0$. This parameter counting argument heuristically explains the large number of tight simplices found in [31].

We tested all cases up to dimension $n = 8$, using our own software to search for numerical solutions and also comparing with the numerical results of Conway, Hardin and Sloane [31]. As with simplices in projective spaces, sometimes the system specified by Proposition 6.3 was singular, and sometimes the numerical evidence was unclear (as we saw in Tables 4 and 6, respectively). These cases are in the third and fourth columns, respectively, of Table 10.

(m,n)	Proven	Singular Jacobian	Ambiguous
$(2,4)$	4–6	2, 3, 7, 8, 10	
$(2,5)$	5–10	4, 11	
$(2,6)$	5–14	3, 4	
$(3,6)$	5–16	2–4	17
$(2,7)$	6–17		18
$(3,7)$	5–22	4, 28	23
$(2,8)$	6–21	4, 5, 28	
$(3,8)$	5–28	4	
$(4,8)$	5–30	2–4	

Table 10: Tight Grassmannian simplices in $G(m,n)$.

In addition to our existence proofs and the previously known explicit constructions, several Grassmannian tight simplices can be proven to exist using the following observation: if there is a tight N–point simplex in $G(m,n)$ for some m,n, then there is a tight N–point simplex in $G(km,kn)$ for all $k \geq 1$. This is immediate from block repetition [33, Proposition 12]. It proves existence for 11 of the singular cases in Table 10. This leaves us with only 7 hitherto unresolved cases in which there is strong numerical evidence for a tight simplex: 4–point simplices in $G(2,5)$, $G(3,6)$, $G(3,7)$ and $G(3,8)$; 7– and 8–point simplices in $G(2,4)$; and 11–point simplices in $G(2,5)$. For completeness, we will settle all of these in the following subsection.

We anticipate no difficulty in applying our techniques to complex or quaternionic Grassmannians, but we have not done so.

6.1 Miscellaneous special cases in Grassmannians

We begin with the case of 11–point tight simplices in $G(2,5)$. This can be handled in the same way as 13–point tight simplices in $\mathbb{HP}^2$ and 25–point tight simplices in $\mathbb{OP}^2$; specifically, we can prove existence of simplices with cyclic symmetry. We will state the analogous result in greater generality than we attempted in Proposition 4.8 (which was written in the special case of $\mathbb{HP}^2$ rather than a general projective space $\mathbb{HP}^{d-1}$), at the cost of some additional complexity.

Proposition 6.5 *Fix dimensions $n > m > 0$ and let σ be the cyclic-shift automorphism $\sigma(x_1, x_2, \dots, x_n) = (x_2, \dots, x_n, x_1)$ on $\mathbb{R}^n$. Set $N = nk+1$ and suppose we have vectors $\{x_{i,j} \in \mathbb{R}^n\}_{i=1,\dots,nk;\, j=1,\dots,m}$. Define $\Pi_i = \sum_{j=1}^m x_{i,j} x_{i,j}^t$ for each i, and $\Pi_N = (Nm/n) I_n - \sum_{i<N} \Pi_i$. Suppose that for some $\eta \in (m/(m+1), m/(m-1))$, the following conditions are satisfied:*

(a) $x_{k+i,j} = \sigma(x_{i,j})$ *for all* $i \le (n-1)k$ *and all* j,

(b) $|x_{i,j}| = 1$ *for all* $i \le k$ *and all* j,

(c) *for all* $i \le k$ *and all* $j < j'$, $\langle x_{i,j}, x_{i,j'}\rangle = 0$,

(d) *the inner products* $\langle \Pi_i, \Pi_{i'}\rangle$ *are all equal for:* (i) $i \le k$, $i' = i + qk$, *and* $q = 1, \dots, \lfloor \frac{n}{2} \rfloor$; (ii) $i \le k-1$, $i' = i_0' + qk$, $i < i_0' \le k$, *and* $q = 0, \dots, n-1$, *and*

(e) *the first* $\lfloor \frac{n}{2} \rfloor + 1$ *entries in the first row of* $\Pi_N^2 - \eta\Pi_N$ *are all zero.*

Then $\eta = 1$, Π_N *is a projection matrix of rank* m, *and the projection matrices* $\{\Pi_i\}_{i \le N}$ *determine a tight* N*–point simplex in* $G(m,n)$.

Proof The automorphism σ of $\mathbb{R}^n$ determines an automorphism of $G(m,n)$ by acting simultaneously on basis vectors, and this latter automorphism is an isometry. The first condition states that the planes spanned by $\{x_{i,1}, \dots, x_{i,m}\}$ and $\{x_{k+i,1}, \dots, x_{k+i,m}\}$ are related by this isometry; thus, taking all $i < N$, we have k orbits under the cyclic-shift action, each of size n. The next two conditions ensure that the matrices Π_i for $i < N$ are orthogonal projections of rank m. Thus the inner products amongst them determine distances in $G(m,n)$. Now, by applying the cyclic-shift isometry we see that the fourth condition is sufficient to force $\{\Pi_i\}_{i<N}$ to determine a regular simplex. Let $\alpha = \langle \Pi_i, \Pi_{i'}\rangle$ be its common inner product.

Consider now the matrix Π_N. It is symmetric, being a linear combination of symmetric matrices. Moreover, it is cyclic-symmetric, since $\sum_{i<N} \Pi_i$ is a sum over orbits of the cyclic shift. It follows that $\Pi_N^2 - \eta\Pi_N$ also shares these properties. Now a matrix with cyclic symmetry is determined by its first row, as the other rows are just shifts thereof. A matrix which is also symmetric is determined by the first $\lfloor \frac{n}{2} \rfloor + 1$ entries in the first row. Therefore, by the last condition, $\Pi_N^2 - \eta\Pi_N = 0$.

It follows that the eigenvalues of Π_N are all either 0 or η. Let r be the rank of Π_N, so that $\operatorname{Tr}\Pi_N = r\eta$. But, since $\operatorname{Tr}\Pi_i = m$ for all $i < N$, we have $\operatorname{Tr}\Pi_N = m$. Hence $\eta = m/r$ is m times the reciprocal of an integer. The assumption that $\eta \in (m/(m+1), m/(m-1))$ then forces $\eta = 1$, from which we conclude that Π_N is an orthogonal projection matrix of rank m.

Now we check that $\langle \Pi_i, \Pi_N\rangle = \alpha$ for all $i < N$. Since $\langle \Pi_i, \Pi_i\rangle = m$ for all i,

$$\Pi_N = \frac{Nm}{n} I_n - \sum_{i<N} \Pi_i, \tag{6-4}$$

and $\langle \Pi_i, \Pi_{i'}\rangle = \alpha$ for distinct $i, i' \le N-1$, we see that $\langle \Pi_N, \Pi_i\rangle$ is independent of i. Let β be this common value. Taking the inner product of (6-4) with Π_N and $\Pi_{i'}$, we obtain, respectively,

$$m = \frac{Nm^2}{n} - (N-1)\beta \quad \text{and} \quad \beta = \frac{Nm^2}{n} - (N-2)\alpha - m.$$

Subtracting and canceling the (nonzero) factor of $N-2$ yields $\alpha = \beta$. Thus, we have a regular simplex, which is tight by (6-4). □

Note that the plane with projection matrix Π_N is the unique plane completing $\{\Pi_i\}_{i<N}$ into a tight simplex. This plane is a fixed point for the cyclic-shift action.

In our case of interest we found a point in which the conditions given in Proposition 6.5 are nonsingular. This yields the following.

Theorem 6.6 *There exists a tight* 11*–point simplex in* $G(2,5)$*. In fact, there is such a tight simplex with cyclic symmetry.*

We remark in passing that every approximate 11–point tight simplex in $G(2,5)$ we found numerically exhibited a symmetry group conjugate to the cyclic symmetry discussed here. With this evidence as well as the fact that $r(11, G(2,5)) = -2 < 0$, we conjecture that every tight 11–point simplex in $G(2,5)$ has a nontrivial symmetry group.

We will settle the remaining cases with algebraic constructions. The four cases of 4–point simplices afford constructions using only rationals and quadratic irrationals, so we give them explicitly here. Given the provided matrices, the proof of the following theorem consists only of a straightforward calculation.

Theorem 6.7 *The four* 2×5 *matrices in Figure 1 are generator matrices whose corresponding planes form a tight simplex in* $G(2,5)$*; in other words, they have orthonormal rows and the spans of those rows constitute a tight simplex. Similarly, the matrices in Figures 2, 3 and 4 determine tight simplices in* $G(3,6)$*,* $G(3,7)$ *and* $G(3,8)$ *respectively.*

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{1}{5}\begin{pmatrix} -\sqrt{3} & 2 & \sqrt{6} & 2\sqrt{3} & 0 \\ 0 & \sqrt{3} & -\sqrt{2} & 0 & \sqrt{20} \end{pmatrix}$$

$$\frac{1}{5}\begin{pmatrix} 3 & 0 & 0 & 4 & 0 \\ 0 & 1 & -2\sqrt{6} & 0 & 0 \end{pmatrix} \qquad \frac{1}{5}\begin{pmatrix} \sqrt{3} & 2 & \sqrt{6} & -2\sqrt{3} & 0 \\ 0 & -\sqrt{3} & \sqrt{2} & 0 & \sqrt{20} \end{pmatrix}$$

Figure 1: Generator matrices for a tight 4–point simplex in $G(2,5)$.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

Figure 2: Generator matrices for a tight 4–point simplex in $G(3,6)$.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\frac{1}{7} \begin{pmatrix} 5 & 0 & 0 & 0 & 0 & 2\sqrt{6} & 0 \\ 0 & 3 & 0 & 0 & 2\sqrt{10} & 0 & 0 \\ 0 & 0 & -1 & 4\sqrt{3} & 0 & 0 & 0 \end{pmatrix}$$

$$\frac{1}{7} \begin{pmatrix} 0 & -2\sqrt{2} & 3 & 2\sqrt{3} & 2\sqrt{5} & 0 & 0 \\ -\sqrt{5} & 0 & -2\sqrt{2} & \sqrt{6} & 0 & \sqrt{30} & 0 \\ 0 & -\sqrt{5} & 0 & 0 & -\sqrt{2} & 0 & \sqrt{42} \end{pmatrix}$$

$$\frac{1}{7} \begin{pmatrix} 0 & 2\sqrt{2} & 3 & 2\sqrt{3} & -2\sqrt{5} & 0 & 0 \\ \sqrt{5} & 0 & -2\sqrt{2} & \sqrt{6} & 0 & -\sqrt{30} & 0 \\ 0 & \sqrt{5} & 0 & 0 & \sqrt{2} & 0 & \sqrt{42} \end{pmatrix}$$

Figure 3: Generator matrices for a tight 4–point simplex in $G(3,7)$.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\sqrt{3} \\ 0 & 1 & 0 & 0 & 0 & -\sqrt{3} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$\frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & -\sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 1 & 0 & 0 & 0 & -\sqrt{3} & 0 \end{pmatrix}$$

Figure 4: Generator matrices for a tight 4–point simplex in $G(3,8)$.

We are now left with the cases of 7– and 8–point tight simplices in $G(2,4)$. These cases are more interesting; the simplest explicit coordinates we have been able to find for them require algebraic numbers of degree 4 and 6, respectively. Because of this, instead of presenting the algebraic numbers here we rely on a computer algebra system to (rigorously) verify the calculation. The computational method is discussed in Section 7.4. Here we simply record the result.

Theorem 6.8 *There exist* 7*– and* 8*–point tight simplices in* $G(2,4)$*.*

We remark in passing that $G(2,4)$ contains tight simplices of N points for all $N \leq 10$ (the theoretical maximum) except for $N = 9$. Compared with the other spaces studied in this paper, only the quaternionic and octonionic projective planes have such a wealth of simplices. Note also that there does not seem to exist a tight simplex of size one less than the upper bound in any of these spaces (see Conjectures 4.13 and 5.10).

7 Algorithms and computational methods

We used computer assistance in several different aspects of this work. Our main results involve two different computational steps: finding approximate solutions and then rigorously proving existence of a nearby solution. We also require a method for computing with real algebraic numbers for Theorem 6.8, and we must discuss how to compute stabilizers of simplices and estimate the dimensions of solution spaces. This section describes the algorithms and programs used for each of these tasks.

7.1 Proof certificates

Only the rigorous proof component is needed to verify our main theorems. Therefore, for ease of verification, we provide PARI/GP code that gives a self-contained proof of existence for each case. We chose PARI because it is freely available and has support for multivariate polynomials and arbitrary-precision rational numbers [64]. Our code is relatively simple and straightforward to adapt to other computer algebra systems. It covers cases with a range of matrix sizes, and the running times of the individual existence proofs vary widely. We have been able to complete the full verification in less than a day on a 2015 personal computer.

The existence proofs rely on Theorem 3.1 via Corollary 3.4. In particular, we use the ℓ_∞ norm on the domain and codomain and we apply Lemma 3.3 to bound the variation of the Jacobian over the cube of radius ε. To check the hypotheses of Corollary 3.4, we need to choose $\varepsilon > 0$, the starting point x_0 and a matrix T and then compute the operator norms of T and $Df(x_0) \circ T - \mathrm{id}_{\mathbb{R}^n}$. We provide input files that specify our choices of x_0, presented using rational numbers with denominator 2^{50}, as well as the constraint function f. We then compute T as described later in this section. Computing operator norms is easy, because the $\ell_\infty \to \ell_\infty$ operator norm of a matrix is just the maximum of the ℓ_1 norms of its rows. (This is one of our primary reasons for choosing the ℓ_∞ norm; for many choices of norms, approximating operator norms of matrices is NP-hard [42].) We always use $\varepsilon = 10^{-9}$, so that the conclusion of Corollary 3.4 is that there is an exact solution, each of whose coordinates differs from our starting point by less than 10^{-9}. In other words, the error is less than one nanounit.

These calculations are organized into fourteen files, enumerated in Table 11. All of these files are available from the web page for this article.[7] They can also be obtained by downloading the source files for this paper from the `arXiv.org` e-print archive, where it is paper number `arXiv:1308.3188`. The file `rigorous_proof.gp` implements Corollary 3.4, and `run_all_proofs.gp` then proves our existence results using the remaining files for input. The next ten files in Table 11 describe the constraints in each of our applications (Propositions 4.1, 4.6, 4.8, 4.11, 5.1, 5.3, 5.5, 5.8, 6.3 and 6.5, respectively). Finally, the last two files specify the starting points, in other words, explicit numerical approximations for the simplices.

`rigorous_proof.gp`	`run_all_proofs.gp`		
`hp_general.gp`	`hp2_12.gp`	`hp2_13.gp`	`hp2_15.gp`
`op2_general.gp`	`op2_24.gp`	`op2_25.gp`	`op2_27.gp`
`grass_general.gp`	`grass2_5_11.gp`		
`projective_data.txt`	`grass_data.txt`		

Table 11: Files for proof certificates.

The translation from mathematics to computer algebra code is straightforward, with just a few issues to address. One is that in the cases with cyclic symmetry, some variables are constrained to be equal to others (for example, the coordinates of x_{m+i} are a cyclic shift of those of x_i in Proposition 4.6).[8] Our data files contain all the points, but in the proofs we eliminate these redundant variables for the sake of efficiency. For example, `projective_data.txt` specifies 12 points in $\mathbb{HP}^2$, and `hp2_12.gp` ignores all but the first four of them.

Another issue is that in three cases (Propositions 4.11, 5.8 and 6.5) we require certain quantities to be close to 1. For example, in Proposition 4.11 we need $||x_i|^4 - 1|$ to be at most 10^{-6} for each i. This could easily be checked by direct computation using the 10^{-9} bound for distance from the starting point, but it is simpler to use the following trick. For each i, we add a new variable v_i, add a new constraint $v_i = |x_i|^4$, and

[7] `dx.doi.org/10.2140/gt.2016.20.1289`

[8] Here and in the next paragraph, x_i is not to be confused with the starting point x_0.

initialize v_i to be 1 at the starting point. Then we can conclude that $||x_i|^4 - 1| < 10^{-9}$ in the exact solution with no additional computation.

All that remains is to describe how we compute the approximate right inverse T for use in Theorem 3.1. Let J be the Jacobian $Df(x_0)$, which by assumption has full row rank. A natural choice for T would be the least-squares right inverse $J^t(JJ^t)^{-1}$ of J, but inverting matrices using exact rational arithmetic is slow and the denominators become large. To save time, we approximate $J^t(JJ^t)^{-1}$ using floating-point arithmetic and obtain T by rounding it to a rational matrix with denominator 2^{50}. Once we have T, the proof is then carried out using only exact rational arithmetic and is therefore completely rigorous.

The use of floating-point arithmetic to obtain T raises one concern about reproducibility. Floating-point error depends delicately on how a computation is carried out, so using a different computer algebra system (or even a different version of PARI/GP) might give a slightly different matrix T, which could in principle prevent the proof from being verified. To guarantee reproducibility, we have analyzed how close an approximation to $J^t(JJ^t)^{-1}$ is needed to make the proof work: in each of our existence proofs, every T satisfying $\|T - J^t(JJ^t)^{-1}\| < 10^{-2}$ works. Any floating-point computation to produce T will meet this undemanding bound if the working precision is high enough, and we have found the default PARI precision to be more than sufficient.

To check this bound of 10^{-2}, first suppose we have some matrix T that works in Corollary 3.4. Examining the slack in the corollary's hypotheses gives an explicit bound

$$\delta_0 = \frac{1 - \|T\| \cdot |f(x_0)|/\varepsilon - \|JT - I_n\| - \varepsilon\,|f|d(d-1)\eta^{d-2}\|T\|}{\|J\| + \varepsilon\,|f|d(d-1)\eta^{d-2} + |f(x_0)|/\varepsilon}$$

such that we can replace T with an arbitrary T' satisfying $\|T' - T\| < \delta_0$. Now every T' satisfying

$$\|T' - J^t(JJ^t)^{-1}\| < \delta$$

works as long as $\delta \le \delta_0 - \|T - J^t(JJ^t)^{-1}\|$. We concluded that $\delta = 10^{-2}$ works by examining all of our cases and applying the following lemma to bound the quantity $\|T - J^t(JJ^t)^{-1}\|$ from above.

Lemma 7.1 *Suppose $J \in \mathbb{R}^{n\times m}$ and $T \in \mathbb{R}^{m\times n}$, and let $\|\cdot\|$ denote the operator norm with respect to some choice of norms on $\mathbb{R}^n$ and $\mathbb{R}^m$. If $\|I_n - T^tTJJ^t\| < 1$, then J has full row rank and*

$$\left\|T - J^t(JJ^t)^{-1}\right\| \le \frac{\|TJJ^t - J^t\| \cdot \|T^tT\|}{1 - \|I_n - T^tTJJ^t\|}.$$

Note that this bound is reasonably natural: if $T = J^t(JJ^t)^{-1}$, then $TJJ^t = J^t$ and $T^tTJJ^t = I_n$, so the bound vanishes.

Proof For all $A, B \in \mathbb{R}^{n\times n}$ with $\|I_n - AB\| < 1$, B is invertible and

$$\|B^{-1}\| \le \frac{\|A\|}{1 - \|I_n - AB\|},$$

because we can take

$$B^{-1} = \sum_{i\ge 0} (I_n - AB)^i A.$$

Setting $A = T^tT$ and $B = JJ^t$ shows that JJ^t is invertible (so J has full row rank), and

$$\|(JJ^t)^{-1}\| \le \frac{\|T^tT\|}{1 - \|I_n - T^tTJJ^t\|}.$$

Now combining this estimate with

$$\|T - J^t(JJ^t)^{-1}\| \le \|TJJ^t - J^t\| \cdot \|(JJ^t)^{-1}\|$$

completes the proof. □

Finally, we note in passing that the implementation in `rigorous_proof.gp` of our proof techniques is general enough to apply to a range of problems. For example, we have used it to reproduce the results of [25] and to prove some of the conjectures in [41], such as the existence of a 26–point 6–design in S^2. (Handling all of the conjectures in [41] would require additional ideas, perhaps along the lines of the special-case arguments in Section 4.2 and Section 4.3.)

7.2 Finding approximate solutions

To find approximate solutions we used a new computer package called QNEWTON, which was written by the last-named author and can be obtained from him upon request. QNEWTON consists of a C++ library with a PYTHON front end and is designed to find solutions to polynomial equations over real algebras. Furthermore, QNEWTON can rigorously prove existence of solutions using Theorem 3.1.

We have chosen to use both QNEWTON and PARI/GP because they have different advantages: the PARI/GP code is shorter and easier to check or adapt to other computer algebra systems, while QNEWTON provides a flexible, integrated environment for both computing approximate solutions and proving existence.

After we specify the polynomials and constraints for the problem and an initial point, QNEWTON attempts to find a solution using a damped Newton's method algorithm.

Newton's method converges rapidly in a neighborhood of a solution, but it is ill-behaved away from solutions; thus we damp the steps so that no coordinate changes in a single step by more than a specified upper bound.

Because the codes we seek are energy minimizers, another approach to finding them would have been gradient descent. In practice, we have found that gradient descent is much slower than Newton's method.

In our computations, we used random Gaussian variables for the initial points and a maximum step size of 0.1. Because our variables represent unit vectors, the step size is approximately one order of magnitude less than the natural scale. By using this approach we were able to find a solution in all cases in which we think there should exist one, using just a few different random starting positions. In most cases we found a solution on the first try. These approximate calculations use double-precision floating-point arithmetic, so we can only expect convergence up to an error of approximately 10^{-15}. In all cases this was more than sufficient for our goals of rigorous proof.

Suppose that, as in Theorem 3.1, we are solving for a zero of a function $f\colon \mathbb{R}^m \to \mathbb{R}^n$. Newton's method calls for repeatedly taking steps Δx satisfying $Df(x)\cdot\Delta x = -f(x)$. In particular, we must repeatedly solve linear systems. When $m > n$ the system is underdetermined. Also, $Df(x)$ may fail to be surjective. Hence we need a linear solver tolerant of such problems. QNEWTON uses a *least-squares* solver that treats small singular values of $Df(x)$ as zero; specifically, it uses the DGELSD function in LAPACK [2]. By using such a solver we can handle cases with redundant constraints. This was particularly useful when we were first determining a minimal set of constraints for our problems.

QNEWTON has native support for multiplication in $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ and $\mathbb{O}$. Also, it uses automatic (reverse) differentiation to compute the Jacobian of the constraint function. These two features substantially increase its performance.

The QNEWTON package also has a mechanism for computer-assisted proof using Theorem 3.1. Like the proofs discussed in the previous section, it uses the ℓ_∞ norm on both domain and codomain. However, unlike those proofs, QNEWTON does not use rational arithmetic, nor does it use Lemma 3.3 to control the variation of the Jacobian. Instead it uses *interval arithmetic*.

Interval arithmetic is a standard tool in numerical analysis to control the errors inherent in floating-point computations. The principle is simple: instead of rounding numbers so that they are exactly representable in the computer, we work with intervals that are guaranteed to contain the correct value. For instance, consider a hypothetical computer capable of storing 4 decimal digits of precision. Using floating-point arithmetic,

π would best be represented as 3.142. Using this, if we computed 2π then we would get 6.284, which is obviously not correct. By contrast, interval arithmetic on the same computer would represent π as the interval $[3.141, 3.142]$. Then 2π would be represented by the interval $[6.282, 6.284]$, which does contain the exact value.

It is clear that balls with respect to the ℓ_∞ norm can be naturally represented using interval arithmetic. Thus, in the notation of Theorem 3.1, for each entry of the Jacobian matrix we can easily compute an interval that contains this entry of $Df(x)$ for every $x \in B(x_0, \varepsilon)$. We then compute an interval guaranteed to contain $\|Df(x) \circ T - \mathrm{id}_{\mathbb{R}^n}\|$ for all such x, and an interval guaranteed to contain $1 - \|T\| \cdot |f(x_0)|/\varepsilon$. If the upper bound of the first interval is less than the lower bound of the second interval, then we are assured that Theorem 3.1 applies.

QNEWTON uses the MPFI library to provide support for interval arithmetic [68]. That in turn relies on MPFR, a library for multiple-precision floating-point arithmetic [37]. One of the main problems with interval arithmetic is that the size of the intervals can grow exponentially with the number of arithmetic operations; this problem can be ameliorated by increasing the precision of the underlying floating-point numbers. It was not an issue in our applications, though.

Finally, we remark upon the computation of the matrix T. It is supposed to be approximately a right inverse of $Df(x_0)$, but otherwise we are free in choosing it. In QNEWTON, we compute T much as in the PARI code. First we compute the matrix $Df(x_0)$ approximately, using floating-point arithmetic. Then we find its pseudoinverse (the least-squares right inverse), again using inexact floating-point arithmetic. Finally, we take the result and replace it with intervals of width 0. This approach is fast and, since T need not be the exact pseudoinverse, still gives rigorous results. It is possible to compute $Df(x_0)$ in interval arithmetic and then compute the pseudoinverse in the same way; this is a bad idea, though, because inverting a matrix in interval arithmetic can result in very large intervals.

7.3 Finding stabilizers

In all but one case, namely 5–point simplices in $\mathbb{OP}^2$, our reported local dimension for the moduli space of tight simplices has the dimension of the full symmetry group deducted. That is valid when each simplex in a neighborhood of the point under consideration has finite (zero-dimensional) stabilizer. This is an open condition and thus only needs to be checked at that single point. We checked this condition by (i) finding a basis for the Lie algebra of the symmetry group, (ii) applying each element of that basis to the points of the simplex to produce tangent vectors, and (iii) verifying that the resulting vectors are linearly independent. In the remainder of this subsection, we explain the calculations in more detail.

The relevant symmetry groups are $\mathrm{Sp}(d)/\{\pm 1\}$ for $\mathbb{HP}^{d-1}$ and F_4 for $\mathbb{OP}^2$, which have dimensions $2d^2+d$ and 52, respectively. Let K be $\mathbb{H}$ or $\mathbb{O}$, as appropriate, and let $\mathfrak{g}$ be the Lie algebra of the isometry group of $K\mathbb{P}^{d-1}$ (in other words, $\mathfrak{g}=\mathfrak{sp}_d$ if $K=\mathbb{H}$ and $\mathfrak{g}=\mathfrak{f}_4$ if $K=\mathbb{O}$).

The Lie algebra $\mathfrak{g}$ acts on the space $\mathcal{H}(K^d)$ of Hermitian matrices. In fact, in this representation it is generated by commutation with traceless skew-Hermitian matrices and application of derivations of the underlying algebra $\mathbb{H}$ or $\mathbb{O}$ (see [10]). The Lie algebra of the stabilizer of the simplex annihilates the projection matrices for the simplex. Thus, if the dimension of the $\mathfrak{g}$–orbit in $\mathcal{H}(K^d)^N$ of an N–point simplex is at least D, then the dimension of the stabilizer is at most $\dim_{\mathbb{R}}\mathfrak{g}-D$.

It remains to compute a lower bound for the dimension of the $\mathfrak{g}$–orbit of the simplex determined by unit vectors $x_1,\dots,x_N\in K^d$. However, we do not have explicit vectors for the points in the simplex. Instead, we have approximations $\tilde{x}_1,\dots,\tilde{x}_N\in K^d$. These vectors are ε–approximations under the ℓ_∞ norm with respect to the standard real basis of K^d, where $\varepsilon=10^{-9}$ (see Section 7.1), and we will give a lower bound that holds over the entire ε–neighborhood of $(\tilde{x}_1,\dots,\tilde{x}_N)$. When we refer below to real entries of vectors and matrices, we will use the standard real basis of K; thus, each entry over K comprises $\dim_{\mathbb{R}} K$ real entries.

Before applying $\mathfrak{g}$, we must convert the vectors x_i to projection matrices. To bound the approximation error, note that each real entry of x_i is bounded by 1 in absolute value (since x_i is a unit vector), and thus each real entry of $\tilde{x}_i$ is bounded by $1+\varepsilon$. It follows that the real entries of $\widetilde{\Pi}_i:=\tilde{x}_i\tilde{x}_i^\dagger$ approximate those of the true projection matrices $\Pi_i:=x_ix_i^\dagger$ to within $(2\varepsilon+\varepsilon^2)\dim_{\mathbb{R}} K$, because each entry over K is just a product in K (so each real entry is the sum of $\dim_{\mathbb{R}} K$ real products), and

$$|uv-\tilde{u}\tilde{v}|\le|u-\tilde{u}|\cdot|v|+|\tilde{u}|\cdot|v-\tilde{v}| \tag{7-1}$$

for $u,v,\tilde{u},\tilde{v}\in\mathbb{R}$.

To understand the action of $\mathfrak{g}$ on $\Pi_1,\dots,\Pi_N$, we begin by choosing a basis of $\mathfrak{g}$. For each basis element, applying it to each of $\Pi_1,\dots,\Pi_N$ and then concatenating the real entries of these N Hermitian matrices yields a single vector of dimension $k:=Nd^2\dim_{\mathbb{R}} K$. The resulting vectors form a $(\dim_{\mathbb{R}}\mathfrak{g})\times k$ real matrix M, and the rank of M is the dimension of the $\mathfrak{g}$–orbit. Of course, the difficulty is that all we can compute is the approximation $\widetilde{M}$ to M obtained from $\widetilde{\Pi}_1,\dots,\widetilde{\Pi}_N$. Each entry of $\widetilde{M}$ is within δ of the corresponding entry of M, where δ is $(2\varepsilon+\varepsilon^2)\dim_{\mathbb{R}} K$ times the greatest $\ell_\infty \to \ell_\infty$ operator norm (with respect to the standard real basis of $\mathcal{H}(K^d)$) of any basis element of $\mathfrak{g}$.

Lemma 7.2 *Let M and $\widetilde{M}$ be $m \times k$ real matrices whose entries differ by at most δ. Then the rank of M is at least the number of eigenvalues of $\widetilde{M}\widetilde{M}^t$ that are greater than $mk\delta(2\max_{i,j}|\widetilde{M}_{i,j}|+\delta)$.*

Proof One can check using (7-1) that the entries of MM^t and $\widetilde{M}\widetilde{M}^t$ differ by at most $\gamma := k\delta(2\max_{i,j}|\widetilde{M}_{i,j}|+\delta)$. Let V be the span of the eigenvectors of $\widetilde{M}\widetilde{M}^t$ with eigenvalues greater than γm. For all $v \in V$ with ℓ_2 norm $|v|_2 = 1$, we have

$$v^t \widetilde{M}\widetilde{M}^t v > \gamma m.$$

On the other hand, $|v|_1 \le \sqrt{m}$ by the Cauchy–Schwarz inequality. Using the observation that

$$|\langle a, b\rangle| \le |a|_1 |b|_\infty \tag{7-2}$$

for vectors a and b, it readily follows that

$$|(MM^t - \widetilde{M}\widetilde{M}^t)v|_\infty \le \gamma\sqrt{m}.$$

Applying (7-2) once more, we obtain

$$|v^t(MM^t - \widetilde{M}\widetilde{M}^t)v| \le \gamma m$$

and hence

$$v^t MM^t v > 0.$$

We have shown that the restriction of MM^t to V is positive definite. Therefore $\operatorname{rank} M = \operatorname{rank} MM^t \ge \dim V$, as desired. □

To apply this lemma, we simply compute the characteristic polynomial of $\widetilde{M}\widetilde{M}^t$. Its roots are the eigenvalues of $\widetilde{M}\widetilde{M}^t$ with multiplicity, and we apply Sturm's theorem to count those that are greater than $mk\delta(2\max_{i,j}|\widetilde{M}_{i,j}|+\delta)$. All of these computations use exact rational arithmetic and thus yield a rigorous lower bound for the rank of M, which is the dimension of the $\mathfrak{g}$–orbit of the simplex $\Pi_1, \dots, \Pi_N$. In other words, they give a rigorous upper bound for the dimension of the stabilizer.

We have implemented these calculations in PARI/GP, and the code can be obtained as described in Section 7.1. The file `apply_lie_basis.gp` sets up the machinery, and `stabilizers.gp` applies it to show that all of the projective simplices we have found have zero-dimensional stabilizers, except for 5 points in $\mathbb{OP}^2$. In that exceptional case, the stabilizer has dimension at most 3. This is good enough because, translated into a dimension for the moduli space of simplices, that bound says that the dimension is at most 0; hence the dimension must equal 0.

7.4 Real algebraic numbers

To verify equations involving algebraic numbers of moderately high degree, we require a computational method for rigorously doing basic arithmetic with such numbers. One possibility is to work in a single number field, but even when each number we manipulate is of manageable degree, the smallest field containing them all may have exponentially high degree. We will instead use the standard approach of "isolating intervals", which is implemented in many modern computer algebra systems. There is no explicit support for the isolating interval method in PARI/GP, so in order to present all of our computer files in one system we provide a short implementation in addition to the pertinent data files for our applications.

The technique is as follows. A real algebraic number α is represented by a triple $(p(x), \ell, u)$, where $p(x)$ is a polynomial with integer coefficients such that $p(\alpha) = 0$, ℓ and u are rational numbers such that $\alpha \in [\ell, u]$, and $p(x)$ has a unique root in the interval $[\ell, u]$ (namely, α). We always take $p(x)$ to be (a scalar multiple of) the minimal polynomial of α, and we use Sturm sequences to rigorously count the number of real roots in a given interval. Given representations $(p_\alpha, \ell_\alpha, u_\alpha)$ and $(p_\beta, \ell_\beta, u_\beta)$ for two real algebraic numbers α, β, we compute a representation for $\alpha + \beta$ by first taking the resultant, in the variable t, of the polynomials $p_\alpha(t)$ and $p_\beta(x-t)$. This gives a polynomial in x for which $\alpha + \beta$ is a root. We then factor the resulting polynomial and count the number of roots for each irreducible factor in the interval $[\ell_\alpha + \ell_\beta, u_\alpha + u_\beta]$. If there is more than one factor that has a root in that interval or some factor has multiple roots, then we bisect the starting intervals $[\ell_\alpha, u_\alpha]$ and $[\ell_\beta, u_\beta]$, using Sturm sequences for p_α and p_β to choose the halves containing α and β, respectively. After a finite number of steps we are left with a valid representation for $\alpha + \beta$. Computing a representation for $\alpha \cdot \beta$ proceeds similarly, beginning with the resultant of $p_\alpha(t)$ and $t^{\deg p_\beta} p_\beta(x/t)$.

Using this system, we can now elucidate the proof of existence for 7– and 8–point tight simplices in $G(2,4)$.

Proof of Theorem 6.8 We provide isolating interval representations for the entries of the 4×4 projection matrices $\Pi_1, \dots, \Pi_N$ for the $N = 7$ or 8 points in each simplex. To verify the construction we need only perform a few calculations. First we need to check that each provided matrix Π satisfies $\Pi = \Pi^t$, $\Pi^2 = \Pi$ and $\operatorname{Tr} \Pi = 2$, as together these conditions imply that Π is an orthogonal projection onto a plane.

Then we just need to verify that $\operatorname{Tr} \Pi_i \Pi_j = (N-2)/(N-1)$ for $i < j \leq N$. These calculations are straightforward given our implementation of the isolating interval method. □

The computer files can be obtained as described in Section 7.1. The file `rtrip.gp` implements isolating intervals ("rtrip" refers to the representation of real algebraic numbers using triples). Using this implementation, `G2_4_verify.gp` carries out the computations with projection matrices taken from `G2_4_data.txt`.

7.5 Estimating dimensions

In Conjectures 4.10, 5.7 and 8.4, we conjecture the dimension of certain solution spaces; here we describe the basis for those conjectures.

Suppose, as is the case in our examples, that we are studying the zero set Z of some function f. Suppose moreover that we have a procedure for converging to zeros of f, using, for example, Newton's method with least-squares solving to handle degeneracy. Thus we have the ability to generate points on Z, and we wish to use that ability to calculate its dimension. This is a simple instance of *manifold learning*, the problem of describing a manifold given sample points embedded in some higher-dimensional space.

For our purposes we use following heuristic. Fix $\varepsilon > 0$. Starting with a solution x_0, we compute N nearby solutions $x_1, \dots, x_N$ as follows. We first set $x_i' = x_0 + \varepsilon g_i$, where g_i is a vector of standard normal random variables, and then use our iterative solver to find a zero x_i of f near x_i'. To first order in ε, the vectors $(x_i - x_0)/|x_i - x_0|$ are random (normalized) samples from the tangent space of Z at x_0. We then form the matrix whose rows are those N vectors and compute its singular values. There should be d singular values of order approximately 1, where d is the dimension of Z. The remaining singular values should be smaller by a factor of ε.

This procedure is certainly not rigorous, but in suitably nice cases, and with proper choice of parameters, one can have a fair amount of confidence in the result. In particular, N should be at least as large as the dimension d, and ε should be chosen small enough that in a ball of radius ε, Z is well-approximated by its tangent space. One pitfall to avoid is that, while ε needs to be small for the tangent space approximation, it should also be large enough that the precision of the solver is better than (approximately) ε^2. If this is violated then we may erroneously identify extra null vectors of $Df(x_0)$ as elements of the tangent space.

In our applications we used $N = 1000$ and $\varepsilon = 10^{-3}$ and we required that Newton's method converge to within 10^{-12}. It was usually easy to identify the jump in singular values after the d corresponding to the tangent space. For instance, Conjecture 4.10 says that, before accounting for overcounting and symmetries, we conjecture a 66–dimensional space of 12–point tight simplices in $\mathbb{HP}^2$. This is based on the following observation: when we ran the procedure just discussed, the first 66 singular values were all in the interval $[2,6]$, but the 67^{th} was 0.04139564.

Remark 7.3 Based on similar computations, we conjecture that the moduli space of SIC-POVMs, simplices of d^2 points in $\mathbb{CP}^{d-1}$, has dimension 1 when $d=3$, and 0 when $d \geq 4$. In particular, we conjecture that, except in $\mathbb{CP}^2$, SIC-POVMs are isolated. This is in accordance with the numerical results in [69], although they searched only for SIC-POVMs that are invariant under the Weyl–Heisenberg group.

8 Explicit constructions

With the exception of Theorems 6.7 and 6.8, all of the new results we have presented so far involve computer-assisted proofs using Theorem 3.1. This allowed us to sidestep explicit constructions, and it also gave local dimensions as a collateral benefit. When an explicit construction is available, though, it can sometimes give insight not proffered by a general existence theorem. We conclude the paper with a few examples of this.

8.1 Two universal optima in SO(4)

Most results in the literature concerning universal optima in continuous spaces are set in two-point homogeneous spaces, that is, spheres and projective spaces. We have already seen another family of spaces (namely, real Grassmannians) but there are many others.

Consider the special orthogonal group $\mathrm{SO}(n)$, endowed with the chordal distance $d_c(U_1,U_2) = \|U_1 - U_2\|_F$ coming from the embedding $\mathrm{SO}(n) \hookrightarrow \mathbb{R}^{n^2}$ as $n \times n$ matrices equipped with the Frobenius norm. This is not the Killing metric, but it has the advantage that its square is a smooth function on $\mathrm{SO}(n) \times \mathrm{SO}(n)$. Note that every element of $\mathrm{SO}(n)$ has norm n, so up to this scaling factor we have an embedding into S^{n^2-1}.

By a *universally optimal* code in $\mathrm{SO}(n)$, we mean a code that minimizes energy for every completely monotonic function of squared chordal distance (see [29]). In this section we present two particularly attractive universal optima in $\mathrm{SO}(4)$.

Theorem 8.1 *There is a 17–point code in* $\mathrm{SO}(4)$ *with the following properties: it is a regular simplex, it is universally optimal, and it has a transitive symmetry group. Moreover, there is no larger regular simplex in* $\mathrm{SO}(4)$.

Proof Given $a, b \in \mathbb{Z}/17\mathbb{Z}$, define the rotation matrix

$$R_{a,b} = \begin{pmatrix} \cos(a\theta) & -\sin(a\theta) & 0 & 0 \\ \sin(a\theta) & \cos(a\theta) & 0 & 0 \\ 0 & 0 & \cos(b\theta) & -\sin(b\theta) \\ 0 & 0 & \sin(b\theta) & \cos(b\theta) \end{pmatrix},$$

where $\theta = 2\pi/17$. For any a, b, c, d, not all zero, the map $\sigma_{a,b,c,d}\colon \mathrm{SO}(4) \to \mathrm{SO}(4)$ defined by $X \mapsto R_{a,b} X R_{c,d}$ is an isometry of $\mathrm{SO}(4)$ of order 17. Set

$$X_0 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \in \mathrm{SO}(4),$$

and let $\{X_i = R_{1,3}^i X_0 R_{4,5}^i\} \in \mathrm{SO}(4)$ be the orbit of X_0 under $\sigma_{1,3,4,5}$. This is a 17–point code which, by construction, has a transitive symmetry group. Moreover, direct calculation shows that it forms a regular simplex.

By virtue of the Euclidean embedding $\mathrm{SO}(4) \hookrightarrow S^{15}$, there can be no regular simplices of more than 17 points, and a 17–point regular simplex must be universally optimal (indeed, it is even universally optimal as a code on the sphere). That proves the remaining claims of the theorem. □

Theorem 8.2 *There is a* 32*–point code in* $\mathrm{SO}(4)$ *with the following properties: it is a subgroup, it is universally optimal, and it forms the vertices of a cross polytope in* S^{15}.

Proof The code consists of all matrices of the form

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix}, \quad \begin{pmatrix} 0 & a & 0 & 0 \\ b & 0 & 0 & 0 \\ 0 & 0 & 0 & c \\ 0 & 0 & d & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & a & 0 \\ 0 & 0 & 0 & b \\ c & 0 & 0 & 0 \\ 0 & d & 0 & 0 \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} 0 & 0 & 0 & a \\ 0 & 0 & b & 0 \\ 0 & c & 0 & 0 \\ d & 0 & 0 & 0 \end{pmatrix},$$

where $a, b, c, d = \pm 1$, with an even number of -1 entries. In other words, we use signed permutation matrices in which the underlying permutation is either trivial or a product of disjoint 2–cycles and the number of minus signs is even. It is not difficult to check that this defines a subgroup of $\mathrm{SO}(4)$.

The supports of these four types of matrices are disjoint, so the corresponding points in $\mathbb{R}^{16}$ are orthogonal. The inner product between two matrices of the same type is simply the inner product of the vectors (a, b, c, d), which is 0 or ± 4 because of the even number of -1 entries. Thus, the code forms a cross polytope in S^{15}.

As in Theorem 8.1, universal optimality of $\mathcal{C}$ in $\mathrm{SO}(4)$ follows from universal optimality as a subset of S^{15} (see [29]). □

8.2 39 points in $\mathbb{OP}^2$

Theorem 8.3 *There exists a tight code $\mathcal{C}$ of 39 points in $\mathbb{OP}^2$. It consists of 13 orthogonal triples, such that $\rho(x_i, x_j) = \sqrt{2/3}$ for any two points x_i, x_j in distinct triples. In other words, if Π, Π' are the projection matrices corresponding to two distinct points in $\mathcal{C}$, then $\langle \Pi, \Pi' \rangle$ equals 0 if the two points are in the same triple and otherwise equals $\frac{1}{3}$.*

Proof First we recall from [32, page 127] the standard construction of a 12–point universal optimum in $\mathbb{CP}^2$: in terms of unit length representatives, it consists of the standard basis

$$(1,0,0),\ (0,1,0),\ (0,0,1)$$

together with the 9 points

$$\frac{1}{\sqrt{3}}(1, \omega^a, \omega^b), \tag{8-1}$$

where $\omega = e^{2\pi i/3}$ and $a, b = 0, 1, 2$.

To construct the desired code, we will use the standard basis together with four rotated copies of (8-1). More precisely, let $\{1, i, j, k\}$ be the standard basis of $\mathbb{H}$ and let ℓ be any one of the remaining four standard basis elements of $\mathbb{O}$. We identify $\omega \in \mathbb{C}$ as an element of $\operatorname{span}\{1, i\} \subset \mathbb{O}$. Set $n = j\ell$. Then we define $\mathcal{C} \subset \mathbb{OP}^2$ to be the code obtained from the standard basis and the points

$$\begin{aligned} &\frac{1}{\sqrt{3}}(1, \omega^a, \omega^b), && \frac{1}{\sqrt{3}}(1, \omega^a j, \omega^b \ell), \\ &\frac{1}{\sqrt{3}}(1, \omega^a \ell, \omega^b n), && \frac{1}{\sqrt{3}}(1, \omega^a n, \omega^b j) \end{aligned} \tag{8-2}$$

for $a, b = 0, 1, 2$. Direct computation shows that this code has the desired distances. In particular, the code splits into 13 distinguished triples of points: the standard basis yields one such triple, and each of the four types of points in (8-2) yields three triples according to the value of $a + b$ modulo 3.

The sums over $\mathcal{C}$ of the first and second harmonics

$$P_1^{(7,3)}(2t-1) = 12t - 4 \quad \text{and} \quad P_2^{(7,3)}(2t-1) = 91t^2 - 65t + 10$$

of $\mathbb{OP}^2$ both vanish; thus $\mathcal{C}$ is a 2–design. Since it has only two inner products between distinct points, and one of those is 0, it is tight [56] and in fact universally optimal [29]. □

The code $\mathcal{C}$ in Theorem 8.3 is a system of 13 mutually unbiased bases. It follows easily from linear programming bounds that it is the largest such system possible in $\mathbb{OP}^2$.

This code is not unique: we can deform it to a four-dimensional family of tight codes by replacing ℓ, n, n and j in the second line of (8-2) with $\xi_1\ell$, $\xi_2 n$, $\xi_3 n$ and $\xi_4 j$, where $\xi_1, \dots, \xi_4$ are complex numbers of absolute value 1. The group of isometries of $\mathbb{OP}^2$ fixing the remaining 21 unchanged points is zero-dimensional (see Section 7.3, for instance), so we have a four-dimensional family even modulo the action of the isometry group F_4 of $\mathbb{OP}^2$. We think the actual space of tight codes is much larger, though. On the basis of numerical evidence (see Section 7.5), we conjecture the following.

Conjecture 8.4 *In a neighborhood of the code constructed in* (8-2)*, the space of tight* 39*–point codes, modulo the action of* F_4*, is a manifold of dimension* 24*.*

At present this remains just a conjecture, though, as we have been unable to identify a nonsingular system of equations to which we can apply Theorem 3.1.

The existence of a code of this form was conjectured by Hoggar [44, Table 2] after classifying the permissible parameters for strongly regular graphs. Excepting a hypothetical 26–point tight simplex, which we conjecture does not exist, there are no remaining cases in which the existence of a tight code in $\mathbb{OP}^2$ is conjectured but not resolved. In fact, based on computations of optimal quasicodes (two-point correlation functions subject to linear programming bounds [30]), we are confident there are no other tight codes in $\mathbb{OP}^2$ with at most 10^4 points. We believe there are no more of any size.

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