

Geometric Properties of Grassmannian Frames for \mathbb{R}^2 and \mathbb{R}^3

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Abstract—Grassmannian frames are frames satisfying a min-max correlation criterion. We translate a geometrically intuitive approach for two and three dimensional Euclidean space (\mathbb{R}^2 and \mathbb{R}^3) into a new analytic method which is used to classify many Grassmannian frames in this setting. The method and associated algorithm decrease the maximum frame correlation, and hence give rise to the construction of specific examples of Grassmannian frames. Many of the results are known by other techniques, and even more generally, so that this paper can be viewed as tutorial. However, our analytic method is presented with the goal of developing it to address unresolved problems in d -dimensional Hilbert spaces which serve as a setting for spherical codes, erasure channel modeling, and other aspects of communications theory

I. INTRODUCTION

A finite frame $\{x_k\}_{k=1}^N \subseteq \mathbb{R}^d$, where \mathbb{R}^d is d -dimensional Euclidean space, is characterized by the property that its span is \mathbb{R}^d , see [1]. The norm $\|x\|$ of $x \in \mathbb{R}^d$ is the usual Euclidean distance. Given a finite frame for \mathbb{R}^d with N elements, we would like to measure the correlation between frame elements, and in particular to decide when the correlation is small. We consider the following metric which is similar to an ℓ^∞ norm [2].

Definition I.1. Let $N \geq d$ and let $X_d^N = \{x_k\}_{k=1}^N$ be a subset of \mathbb{R}^d with each $\|x_k\| = 1$. The *maximum correlation* of X_d^N , $\mathcal{M}_\infty(X_d^N)$, is defined as

$$\mathcal{M}_\infty(X_d^N) = \max_{k \neq l} |\langle x_k, x_l \rangle|.$$

Note that because we consider the absolute value of the inner product rather than just the inner product, if the angle between a pair of vectors is closer to 90° , then the pair is less correlated, while if the angle is closer to 0° or 180° then the pair is more correlated. Thus, we are measuring the smaller angle between the lines (one dimensional subspaces) spanned by these vectors. We could instead consider an ℓ^1 , ℓ^2 , or ℓ^p -type norm to measure correlation, i.e.,

$$\mathcal{M}_p(X_d^N) = \left(\sum_{k \neq l} |\langle x_k, x_l \rangle|^p \right)^{1/p}, \quad (\text{I.1})$$

or even weighted versions of (I.1). (See [3] for a discussion of the case $p = 1, 2$.)

Fix d and N with $N \geq d$. Our goal is to construct N element unit norm frames, X_d^N , with smallest maximum correlation, $\mathcal{M}_\infty(X_d^N)$, i.e., unit norm frames that are maximally spread apart. To this end we make the following definition.

Definition I.2. Let $N \geq d$. A sequence $U_d^N = \{u_k\}_{k=1}^N \subseteq \mathbb{R}^d$ of unit norm vectors is an (N, d) -Grassmannian frame if it is a frame and if

$$\mathcal{M}_\infty(U_d^N) = \inf \{ \mathcal{M}_\infty(X_d^N) \}, \quad (\text{I.2})$$

where the infimum is taken over all unit norm, N -element frames for \mathbb{R}^d .

A compactness argument shows that Grassmannian frames exist (see Appendix A), but constructing Grassmannian frames is challenging [4], [5], [6]. As is described in [2], the concept of Grassmannian frames is related to several other areas of mathematics and engineering, for example, packings in Grassmannian spaces, spherical codes and designs, the construction of equiangular lines, strongly regular graphs, and reduction of losses associated with packet based communications systems such as the Internet, [7], [8], [9].

In this paper we give an analytic construction of Grassmannian frames in \mathbb{R}^d , when $d = 2, 3$. The first treatment of this construction problem in the case $d = 3$ is found in [10]. There are extensive computational and theoretical results in [4] which approach this construction problem from a sphere packing point of view. The relevance of such constructions was brought to the attention of the frame community in [2].

After stating some technical preliminaries in Section II, we characterize all $(N, 2)$ -Grassmannian frames in Section III. In Section IV we state and prove a modest generalization of a theorem, given in [2], which provides a lower bound for $\mathcal{M}_\infty(X_d^N)$. Section V is devoted to the construction of $(4, 3)$ -Grassmannian frames from first principles rather than using the theorem in Section IV. Convexity arguments are used in Section VI to construct examples of $(5, 3)$ -Grassmannian frames. In Section VII, we construct a $(6, 3)$ -Grassmannian frame using the theorem in Section IV. The techniques used in the constructions of Sections V, VI, and VII were developed in part to fathom the geometrical ideas of Fejes-Tóth [10].

Our presentation is technical, and, we believe, necessarily so. Some of the technicalities are routine, but they are included since going from one step to the next without exhibiting them sometimes seemed mysterious. On the other hand, some of our techniques may very well be useful in developing more general methods of finding frames with small correlations in applicable complex and higher dimensional settings. For example, see the new techniques used in proving Propositions VI.3 and VI.4,

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and Lemmas VI.5 and VI.6. Our notation is standard, but we do mention that “ \implies ” means “implies” and “ \iff ” means “if and only if”.

II. PRELIMINARIES

In this section, we collect some definitions and theorems used in the sequel.

The *transpose* of a vector or matrix A is denoted by A^T ; and the *Hermitian transpose* of a vector or matrix B with complex entries is denoted by B^* , the conjugate transpose of B , i.e., $B^* = \overline{B^T}$. A $d \times d$ matrix U with real entries is *orthogonal* if the columns of U are orthonormal, i.e., $U^T U = I_d$, where U^T is the transpose of U and I_d is the $d \times d$ identity matrix. If U is orthogonal, i.e., $U \in SO_d$, then for any $x, y \in \mathbb{R}^d$, $\|Ux\| = \|x\|$ and $\langle Ux, Uy \rangle = \langle x, y \rangle$.

The *torus* is $\mathbb{T}_{2\pi} = \mathbb{R}/(2\pi\mathbb{Z})$. We take any fixed half-open interval of length 2π to be a representative of $\mathbb{T}_{2\pi}$.

The *unit sphere* in \mathbb{R}^d is $S^{d-1} = \{x \in \mathbb{R}^d : \|x\| = 1\}$. A set $\{x_1, \dots, x_N\}$ of unit norm vectors is *equiangular* if there is an $\alpha \in [0, 1]$ such that $|\langle x_k, x_l \rangle| = \alpha$ when $k \neq l$.

A $d \times d$ matrix A with real entries is *symmetric* if $A^T = A$.

The spectral theorem for symmetric matrices is the following, see [11]. We use it in Theorem IV.2.

Theorem II.1 (Spectral theorem). *A $d \times d$ symmetric matrix A over \mathbb{R} has the following properties:*

- i. *A has d real eigenvalues counting multiplicities.*
- ii. *The dimension of the eigenspace for each eigenvalue λ equals the multiplicity of λ as a root of the characteristic equation $\det(A - \lambda I) = 0$.*
- iii. *The eigenspaces are mutually orthogonal, in the sense that eigenvectors corresponding to different eigenvalues are orthogonal.*
- iv. *A is orthogonally diagonalizable, i.e., there is an orthonormal basis of eigenvectors for A .*

We now state some basic definitions of frame theory [12], [3], [13], [14], [1]. Let \mathcal{H} be a separable Hilbert space, and let $X = \{x_n : n \in \mathcal{I}\} \subset \mathcal{H}$ where \mathcal{I} is a countable indexing set. Consider the following map associated with the set X :

$$L : \mathcal{H} \rightarrow \ell^2(\mathcal{I}) \\ y \mapsto \{\langle y, x_n \rangle\}_{n \in \mathcal{I}}.$$

If L is a well-defined linear map, i.e., if $\sum_{n \in \mathcal{I}} |\langle y, x_n \rangle|^2 < \infty$ for any $y \in \mathcal{H}$, then L is a *Bessel map* and X is a *Bessel sequence*. The *adjoint* of L is the map

$$L^* : \ell^2(\mathcal{I}) \rightarrow \mathcal{H} \\ \{c[n]\}_{n \in \mathcal{I}} \mapsto \sum_{n \in \mathcal{I}} c[n]x_n.$$

If L is a Bessel map, the corresponding *frame operator* is the map $S : \mathcal{H} \rightarrow \mathcal{H}$ defined as L^*L . Thus, for any $y \in \mathcal{H}$,

$$S(y) = L^*(L(y)) = \sum_{n \in \mathcal{I}} \langle y, x_n \rangle x_n.$$

As such $y = \sum_{n \in \mathcal{I}} \langle y, x_n \rangle S^{-1}x_n$. The *Grammian operator* is the map $G : \ell^2(\mathcal{I}) \rightarrow \ell^2(\mathcal{I})$ defined as $G = LL^*$. Both S and G are positive, and hence self-adjoint operators.

A Bessel sequence X is a *frame* for \mathcal{H} if there exist constants A, B with $0 < A \leq B < \infty$ such that, for any $y \in \mathcal{H}$,

$$A \|y\|^2 \leq \sum_{n \in \mathcal{I}} |\langle y, x_n \rangle|^2 \leq B \|y\|^2.$$

Thus, given any frame, we have four natural maps: L , L^* , S , and G . If the indexing set \mathcal{I} is finite then X is called a *finite frame*. Also, if $A = B$ then X is called a *tight frame*, or, if we wish to emphasize the bound, an *A-tight frame*.

Throughout this paper we shall use that fact that any finite set of vectors forms a frame for its span with the frame bounds being the largest and smallest eigenvalues of the frame operator. Since any finite set of vectors automatically has an upper frame bound by Cauchy-Schwarz, the fact that any finite set is a frame for its span is a consequence of the following result.

Proposition II.2. *The following three statements are equivalent:*

- i. $\{x_n\}_{n=1}^N$ is a frame for \mathbb{R}^d ;
- ii. $\text{span}\{x_n\}_{n=1}^N = \mathbb{R}^d$.
- iii. $\exists A > 0$ such that $\forall y \in \mathbb{R}^d$,

$$A \|y\|^2 \leq \sum_{n=1}^N |\langle y, x_n \rangle|^2$$

III. TWO DIMENSIONAL GRASSMANNIAN FRAMES

We classify all $(N, 2)$ -Grassmannian frames. The idea for the following proof is illustrated in Figure 1. In fact, in order to maximize the minimum angle between pairs of vectors, the vectors we must be equally spaced.

Theorem III.1 ($(N, 2)$ -Grassmannian). *Let $X = X_2^N = \{x_k\}_{k=1}^N$ be a collection of N unit vectors in \mathbb{R}^2 . Then we have the lower bound*

$$\cos(\pi/N) \leq \mathcal{M}_\infty(X).$$

Furthermore, X is an $(N, 2)$ -Grassmannian frame if and only if there is $P \in SO_2$ and a sequence $\{\varepsilon_k\}_{k=1}^N \subset \{\pm 1\}^N$ such that

$$P(\varepsilon X) := \{P(\varepsilon_k x_k) : x_k \in X_2^N\} \quad (\text{III.1}) \\ = \left\{ \begin{pmatrix} \cos(\pi k/N) \\ \sin(\pi k/N) \end{pmatrix} : k = 1, \dots, N \right\}.$$

Proof: Let $\delta_1 = (1, 0)^T$ and let $\delta_2 = (0, 1)^T$. Since $|\langle x, y \rangle| = |\langle x, -y \rangle|$, we note that changing the sign of any $x_k \in X$ does not effect the value of $\mathcal{M}_\infty(X)$. Thus, by changing the sign on x_k when necessary, we may assume $x_k \in \{v \in S^1 : \langle v, \delta_2 \rangle \geq 0\}$. Also, since rotations preserve inner products, applying a rotation to all the vectors in X does not effect $\mathcal{M}_\infty(X)$. Thus, rotating by $-\phi$, where $\phi = \min_{k=1, \dots, N} \cos^{-1}(\langle x_k, \delta_1 \rangle)$, and reordering if necessary, we may assume $x_1 = \delta_1 = (1, 0)^T$, and

$$1 \geq \langle x_2, x_1 \rangle \geq \langle x_3, x_1 \rangle \geq \dots \geq \langle x_N, x_1 \rangle \geq -1. \quad (\text{III.2})$$

For $k = 1, \dots, N-1$, let θ_k be the angle between x_k and x_{k+1} , and let θ_N be the angle between x_N and the negative x -axis, i.e., $\theta_k = \cos^{-1}(\langle x_{k+1}, x_k \rangle)$ and $\theta_N = \cos^{-1}(\langle -\delta_1, x_N \rangle)$, see Figure 1 for an example when $N = 6$.

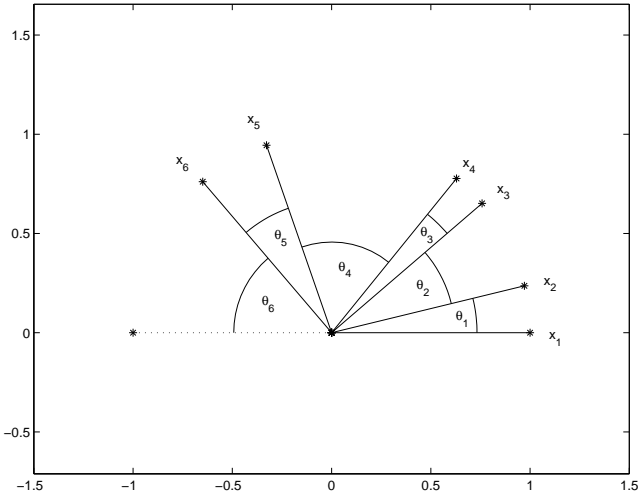


Fig. 1. An example of the reordering induced by the inequalities on the inner products in (III.2) for $N = 6$.

Then, because of the above reordering, $\theta_k \geq 0$ for $k = 1, \dots, N$, and $\sum_{k=1}^N \theta_k = \pi$. Thus, for $1 \leq l < k \leq N$,

$$|\langle x_k, x_l \rangle| = \left| \cos \left(\sum_{j=l}^{k-1} \theta_j \right) \right|,$$

where $\min_{k=1, \dots, N-1} \theta_k \leq \sum_{j=l}^{k-1} \theta_j \leq \pi - \theta_N$.

Furthermore, $|\cos(\theta)|$ has a maximum on $[0, \pi]$ at $\theta = 0$, and $\theta = \pi$, and $|\cos(\theta)|$ is monotone decreasing on $[0, \pi/2]$ and monotone increasing on $[\pi/2, \pi]$. Hence,

$$\begin{aligned} \mathcal{M}_\infty(X) &= \max_{k \neq l} \left| \cos \left(\sum_{j=l}^{k-1} \theta_j \right) \right| \\ &= \max \left\{ |\cos(\pi - \theta_N)|, \left| \cos \left(\min_{k=1, \dots, N-1} \theta_k \right) \right| \right\} \\ &= \left| \cos \left(\min_{k=1, \dots, N} \theta_k \right) \right|. \end{aligned}$$

Therefore, in order to minimize $\mathcal{M}_\infty(X)$ we must choose N positive numbers $\alpha_1, \dots, \alpha_N$ which sum to π and which minimize $|\cos(\min_{k=1, \dots, N} \alpha_k)|$, and, hence, which maximize the expression

$$\min_{k=1, \dots, N} \alpha_k. \quad (\text{III.3})$$

Now we claim that if $\alpha_1, \dots, \alpha_N$ maximize (III.3) then $\alpha_1 = \dots = \alpha_N$. We prove this implication by contraposition, i.e., assume it is not the case that $\alpha_1 = \dots = \alpha_N$. Then there is an $m \in \{1, 2, \dots, N-1\}$ so that if we list $\alpha_1 \leq \dots \leq \alpha_N$ by size, then only the first m are equal, and the $(m+1)$ st is strictly larger than the m th, i.e.,

$$\alpha_{k_1} = \alpha_{k_2} = \dots = \alpha_{k_m} < \alpha_{k_{m+1}} \leq \dots \leq \alpha_{k_N}.$$

Let $\nu = \alpha_{k_{m+1}} - \alpha_{k_m}$ and, for $j = 1, \dots, N$, define the sequence β_{k_j} as

$$\beta_{k_j} = \begin{cases} \alpha_{k_j} + \frac{\nu}{2m} & \text{for } j = 1, \dots, m, \\ \alpha_{k_j} - \frac{\nu}{2} & \text{for } j = m+1, \\ \alpha_{k_j} & \text{for } j = m+2, \dots, N. \end{cases}$$

Now the new set,

$$\beta_{k_1} = \beta_{k_2} = \dots = \beta_{k_m} \leq \beta_{k_{m+1}} \leq \dots \leq \beta_{k_N},$$

has a strictly larger minimum angle than the original since for $j = 1, \dots, N$,

$$\min_{k=1, \dots, N} \alpha_k = \alpha_{k_1} < \alpha_{k_1} + \frac{\nu}{2m} = \beta_{k_1} \leq \beta_j.$$

We see that the original α s do not maximize (III.3). So by contraposition we have that if the α s maximize (III.3), then they must all be equal. Finally, if α is the common value, then $\sum_{k=1}^N \alpha_k = N\alpha = \pi$, and therefore $\alpha = \pi/N$. Thus, $\pi/N \geq \min_{k=1, \dots, N} \theta_k$, and therefore

$$\cos(\pi/N) \leq \cos \left(\min_{k=1, \dots, N} \theta_k \right) = \mathcal{M}_\infty(X).$$

Next we prove that any $(N, 2)$ -Grassmannian frame is, up to a sign change, the first N adjacent vertices of a regular $2N$ -gon. If X is an $(N, 2)$ -Grassmannian frame, then, using the above argument, we see that we can choose $\{\varepsilon_k\} \subset \{\pm 1\}^N$ and $P \in SO_2$ so that the frame

$$P(\varepsilon X) = \{P(\varepsilon_k x_k) : x_k \in X\}$$

is in the closed upper half plane with one of the vectors being $(1, 0)^T$; and

$$\mathcal{M}_\infty(X) = \mathcal{M}_\infty(P(\varepsilon X)) = \cos \left(\min_{k=1, \dots, N} \theta_k \right),$$

where θ_k is the angle between the k th and $(k+1)$ st adjacent vectors in $P(\varepsilon X)$ (reindexing may be necessary). Since an $(N, 2)$ -Grassmannian frame minimizes the ∞ -correlation $\mathcal{M}_\infty(X)$, the above argument also shows that $\theta_1 = \dots = \theta_N = \pi/N$. Therefore, the angle between adjacent vectors in $P(\varepsilon X)$ is π/N , and we have proved the forward direction of the equivalence.

To show the reverse implication we note that if

$$P(\varepsilon X) = \left\{ \begin{pmatrix} \cos(\pi k/N) \\ \sin(\pi k/N) \end{pmatrix} : k = 1, \dots, N \right\},$$

then

$$\begin{aligned} \mathcal{M}_\infty(X) &= \mathcal{M}_\infty(P(\varepsilon X)) \\ &= \cos \left(\min_{k=1, \dots, N} \theta_k \right) = \cos(\pi/N). \end{aligned}$$

Hence, X is $(N, 2)$ -Grassmannian since it achieves the lower bound. Q.E.D.

Notice that for N odd, if we change the sign on the the N th roots of unity below the real axis, then we obtain the frame described in the above claim with $\varepsilon_k = 1$, i.e., with all vectors in the upper half plane, and a common angle of π/N between

adjacent vectors. Hence for N odd, the N th roots of unity are $(N, 2)$ -Grassmannian. Furthermore, for N even, the N th roots of unity do not form an $(N, 2)$ -Grassmannian frame because ζ and $-\zeta$ are both N th roots. If we identify ζ and $-\zeta$ then we obtain an $(N/2, 2)$ -Grassmannian frame.

IV. A LOWER BOUND FOR \mathcal{M}_∞

It is more difficult to construct a Grassmannian frame in \mathbb{R}^3 for $N > 3$ than in \mathbb{R}^2 . Thus, we first derive a lower bound for the maximum correlation between frame elements of an N -element frame for \mathbb{R}^d , see [2], [15] for superb treatments, although we have felt compelled to spell-out all details. Such lower bounds are useful in coding theory [16], and we first learned of them in [2].

The proofs of the following lemma and theorem are found in Appendix B.

Lemma IV.1. *Let H_n be the $n \times n$ matrix with 1 on the main diagonal and β elsewhere, and let C_n be the $n \times n$ matrix defined by*

$$[C_n]_{i,j} = \begin{cases} \beta, & \text{if } (i, j) = (1, 1) \\ [H_n]_{i,j}, & \text{otherwise,} \end{cases}$$

where $[H_n]_{i,j}$ is the (i, j) th entry of the matrix H_n . Then

$$\det(H_n) = (1 + (n-1)\beta)(1-\beta)^{n-1} \quad (\text{IV.1})$$

and

$$\det(C_n) = \beta(1-\beta)^{n-1}. \quad (\text{IV.2})$$

Theorem IV.2. *Let $N \geq d$, let X_d^N be an N -element subset of S^{d-1} , and let $d_0 = \dim(\text{span}(X_d^N))$. Then*

$$\mathcal{M}_\infty(X_d^N) \geq \sqrt{\frac{N-d_0}{d_0(N-1)}}, \quad (\text{IV.3})$$

where equality holds in (IV.3) if and only if

- X_d^N is equiangular, and
- X_d^N is a tight frame for its span with frame bounds $A = B = \frac{N}{d_0}$.

Furthermore, if $N > \frac{d(d+1)}{2}$, then X_d^N is not equiangular, hence equality cannot hold in (IV.3).

Remark: Theorem III.1 shows that $\mathcal{M}_\infty(X_2^N) \geq \cos(\pi/N)$, while Theorem IV.2 shows $\mathcal{M}_\infty(X_2^N) \geq \sqrt{\frac{N-2}{2(N-1)}}$. Using standard calculus techniques, we can show that the equality in Theorem III.1 is an improvement over the bound in Theorem IV.2 for all $N > 3$. Let

$$f(x) = \cos^2(\pi/x) - \frac{x-2}{2(x-1)}$$

(see Figure 2), so that

$$f'(x) = \frac{\pi}{x^2} \sin\left(\frac{2\pi}{x}\right) - \frac{1}{2(x-1)^2}$$

and

$$f''(x) = -\frac{2\pi}{x^3} \left(\frac{\pi}{x} \cos\left(\frac{2\pi}{x}\right) + \sin\left(\frac{2\pi}{x}\right) \right) + \frac{1}{(x-1)^3}.$$

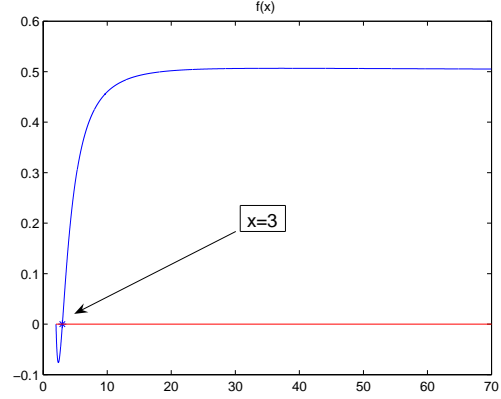


Fig. 2. The function $f(x) = \cos^2(\pi/x) - \frac{x-2}{2(x-1)}$ on $[2, 70]$.

Hence,

$$f'(x) > 0 \iff \sin(2\pi/x) > \frac{1}{2\pi} \left(\frac{x}{x-1} \right)^2.$$

For $x \in [3, 6]$,

$$\sin\left(\frac{2\pi}{x}\right) \geq \frac{\sqrt{3}}{2} \geq \frac{9}{8\pi} \geq \frac{1}{2\pi} \left(\frac{x}{x-1} \right)^2,$$

and so $f(x)$ is increasing for $x \in [3, 6]$; and, since $f(3) = 0$, we have that $f(x) \geq 0$ for $x \in [3, 6]$. Furthermore, for $x \in [6, \infty)$, $\frac{36}{50\pi} \geq \frac{1}{2\pi} \left(\frac{x}{x-1} \right)^2$. Also, $\sin\left(\frac{2\pi}{x}\right) \geq \frac{36}{50\pi}$ if and only if

$$x \leq \frac{2\pi}{\sin^{-1}\left(\frac{36}{50\pi}\right)} < 27.172.$$

Thus, $f(x)$ is increasing for $x \in [3, 27]$, and, hence, it is greater than zero on that same interval. We also note that for $x > 1$,

$$\frac{1}{2\pi} < \frac{1}{2\pi} \left(\frac{x}{x-1} \right)^2.$$

Further, $\sin\left(\frac{2\pi}{x}\right) \leq \frac{1}{2\pi}$ when

$$x \geq \frac{2\pi}{\sin^{-1}\left(\frac{1}{2\pi}\right)} > 39.310.$$

Hence f is decreasing on the interval $[40, \infty)$, and since $\lim_{x \rightarrow \infty} f(x) = \frac{1}{2}$, we have that $f(x) > \frac{1}{2}$ for $x \in [40, \infty)$. Finally, we check that $f'' < 0$ on the interval $[27, 40]$ and $f(27), f(40) > \frac{1}{2}$; thus, $f(x) > \frac{1}{2}$ on $[27, 40]$. In summary we have shown that $f(x) > 0$ on $(3, \infty)$ and that $f(x) > \frac{1}{2}$ on $[27, \infty)$. Therefore,

$$\cos\left(\frac{\pi}{N}\right) > \sqrt{\frac{N-2}{2(N-1)}} \quad \text{for } N > 3,$$

and we see that Theorem III.1 is an improvement over Theorem IV.2 in the case $d = 2$, see Table I.

In light of Theorem IV.2, we make the following definition,

Definition IV.3. Let $N, d \in \mathbb{N}$ with $d \leq N \leq \frac{d(d+1)}{2}$. Let $X_d^N = \{x_k\}_{k=1}^N$ be a frame for \mathbb{R}^d with $\|x_k\| = 1$. We call

N	Optimal bound $= \sqrt{\frac{N-2}{2(N-1)}}$	Bound from Theorem III.1 $\cos(\pi/N)$
3	0.5000	0.5000
4	0.5774	0.7071
5	0.6124	0.8090
6	0.6325	0.8660
7	0.6455	0.9010
8	0.6547	0.9239
9	0.6614	0.9397
10	0.6667	0.9511

TABLE I

IMPROVEMENT OF THE OPTIMAL BOUND DERIVED IN THEOREM IV.2 FOR THE CASE OF $(N, 2)$ -GRASSMANNIAN FRAMES.

N	Optimal bound $= \sqrt{\frac{N-3}{3(N-1)}}$	Grassmannian bound $= \min \mathcal{M}_\infty(X_3^N)$
3	0	0
4	0.3333	0.3333
5	0.4082	0.4472
6	0.4472	0.4472

TABLE II

BOUNDS FOR N -ELEMENT FRAMES IN \mathbb{R}^3 WITH POTENTIAL OF BEING OPTIMAL GRASSMANNIAN.

X_d^N an optimal Grassmannian frame if X_d^N satisfies (IV.3) with equality, i.e.,

$$\mathcal{M}_\infty(X_d^N) = \sqrt{\frac{N-d}{d(N-1)}}.$$

In \mathbb{R}^2 , since $d = 2$ and $\frac{d(d+1)}{2} = 3$, only frames with $N = 2$ and $N = 3$ elements can be optimal Grassmannian. Since $\cos(\pi/2) = 0 = \sqrt{(2-2)/(2(2-1))}$, and $\cos(\pi/3) = 1/2 = \sqrt{(3-2)/(2(3-1))}$, both $(2, 2)$ - and $(3, 2)$ -Grassmannian frames are optimal. The same phenomenon does not happen in three dimensions. Table II lists the Grassmannian bound which will be proven below and the optimal bound for $N = 3, 4, 5, 6$, (the only N s with the possibility of being optimal). By inspecting Table II, we notice that $(5, 3)$ -Grassmannian frames are not optimal, while $(3, 3)$, $(4, 3)$ and $(6, 3)$ -Grassmannians are optimal.

V. $(4, 3)$ -GRASSMANNIAN FRAMES

In this section and the next two, we shall derive the bounds for three dimensional Grassmannian frames with $N = 3, 4, 5$ and 6. First note that if $N = 3$, and if X is any orthonormal basis for \mathbb{R}^3 , then $0 \leq \mathcal{M}_\infty(X) = 0$. Hence, any orthonormal basis is Grassmannian and, in fact, X is trivially optimal Grassmannian.

Next consider $N = 4$. We need the following two lemmas which are necessary to rigorize Fejes Tóth's ideas in [10]. In particular, Lemma V.1 is intuitively elementary when we

consider the fact that the ℓ^2 -norm is convex, Q is convex, and C is the set of extreme points of Q .

Lemma V.1. Let $a \in \mathbb{R}^d$, and let $\{v_1, v_2, \dots, v_d\} \subset \mathbb{R}^d$. Set

$$Q = \left\{ a + \sum_{j=1}^d s_j v_j : s_j \in [0, 1] \right\}$$

$$C = \left\{ a + \sum_{j=1}^d \varepsilon_j v_j : \varepsilon_j \in \{0, 1\} \right\},$$

and choose $c \in C$ such that $\|c\| = \max \{\|c_l\| : c_l \in C\}$ where $l = 1, \dots, 2^d$. Then, for any $v \in Q \setminus C$, $\|v\| < \|c\|$.

Lemma V.1 is used in the proof of Lemma V.2.

Lemma V.2. Let $\{b, y_1, y_2, y_3\} \subset S^2$. If $|\langle b, y_1 \rangle|$, $|\langle b, y_2 \rangle|$, and $|\langle b, y_3 \rangle|$ are not all equal, then there is a constructible $c \in \mathbb{R}^3$ such that

$$\max \{|\langle b, y_k \rangle| : k = 1, 2, 3\} \quad (\text{V.1})$$

$$> \max \left\{ \left| \left\langle \frac{c}{\|c\|}, y_k \right\rangle \right| : k = 1, 2, 3 \right\}.$$

Furthermore, $\left| \left\langle \frac{c}{\|c\|}, y_1 \right\rangle \right| = \left| \left\langle \frac{c}{\|c\|}, y_2 \right\rangle \right| = \left| \left\langle \frac{c}{\|c\|}, y_3 \right\rangle \right|$.

Proof: Case 1. $\{y_1, y_2, y_3\} \subset S^2$ is linearly dependent. Then there is $a_1, a_2, a_3 \in \mathbb{R}^3$ with at least one (actually two) $a_k \neq 0$ such that

$$a_1 y_1 + a_2 y_2 + a_3 y_3 = 0.$$

Therefore $\dim(\ker Y) \geq 1$, where Y is a 3×3 matrix with columns y_j . Hence, $\dim(\text{span } Y) = \text{rank } Y \leq 2$. We can choose $c \in (\text{span } Y)^\perp$, so that

$$\forall k = 1, 2, 3, \quad |\langle b, y_k \rangle| > 0 = \left| \left\langle \frac{c}{\|c\|}, y_k \right\rangle \right|,$$

since by assumption we know that the $|\langle b, y_k \rangle|$ cannot all be equal, and hence cannot all equal zero.

Case 2. $\{y_1, y_2, y_3\} \subset S^2$ is linearly independent. Let Y be the 3×3 matrix whose columns are y_j . Then Y^T is invertible. Let c_1, \dots, c_4 be the columns of the following 3×4 matrix product

$$\begin{bmatrix} c_1 & c_2 & c_3 & c_4 \\ | & | & | & | \end{bmatrix} = (Y^T)^{-1} \begin{bmatrix} 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}, \quad (\text{V.2})$$

see Figure 3. Notice that

$$c_1 = (Y^T)^{-1} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = (Y^T)^{-1} \left(\begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \right)$$

$$= c_2 + c_3 + c_4.$$

Let $c \in \{c_1, \dots, c_4\}$ have the property that $\|c\| = \max \{\|c_1\|, \dots, \|c_4\|\}$. We now show that this procedure of matrix multiplication followed by taking the maximum gives rise to a vector $c \in \mathbb{R}^3$ which satisfies the conclusion of Lemma V.2.

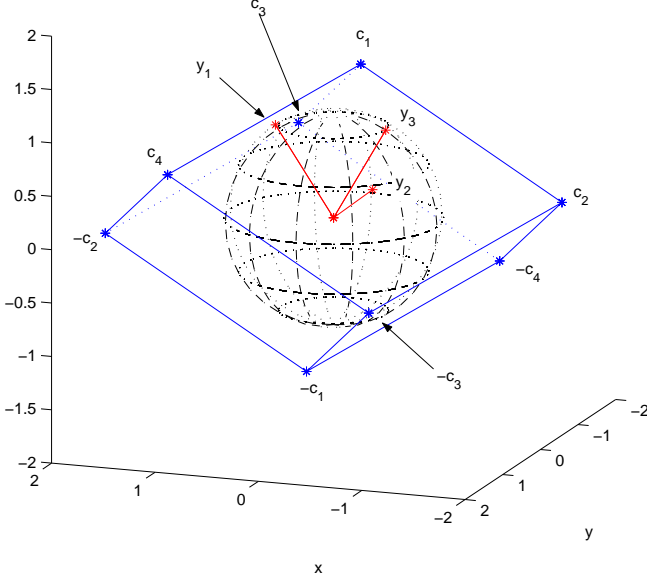


Fig. 3. An example showing the points $\pm c_k$, $k = 1, \dots, 4$, and their relationship to the vectors y_1, y_2, y_3 . Note, y_2 lies on the plane with vertices $\{c_1, c_2, -c_3, c_4\}$.

For $j = 1, 2, 3$, define $v_j = c_{j+1} - c_1$, and, set

$$Q = \left\{ c_1 + \sum_{j=1}^3 s_j v_j : s_j \in [0, 1] \right\}$$

and

$$C = \left\{ c_1 + \sum_{j=1}^3 \varepsilon_j v_j : \varepsilon_j \in \{0, 1\} \right\}.$$

Identify a point in C with a vector $(\varepsilon_1, \varepsilon_2, \varepsilon_3)$. For example, if $(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (1, 0, 1)$, then $v = c_1 + v_1 + v_3$. Observe that since $c_1 = c_2 + c_3 + c_4$, we have the following bijection between C and $\{\pm c_1, \pm c_2, \pm c_3, \pm c_4\}$:

$$\begin{aligned} (0, 0, 0) &\longleftrightarrow c_1 \\ (1, 0, 0) &\longleftrightarrow c_2 \\ (0, 1, 0) &\longleftrightarrow c_3 \\ (0, 0, 1) &\longleftrightarrow c_4 \\ (1, 1, 0) &\longleftrightarrow -c_4 \\ (1, 0, 1) &\longleftrightarrow -c_3 \\ (0, 1, 1) &\longleftrightarrow -c_2 \\ (1, 1, 1) &\longleftrightarrow -c_1. \end{aligned}$$

In particular, $\|c\| = \max \{\|c'\| : c' \in C\}$.

Now, if

$$H = \{v \in \mathbb{R}^3 : |\langle v, y_k \rangle| \leq 1 \text{ for } k = 1, 2, 3\}$$

then $Q = H$. To see this, we check both containments, but first note that (V.2) with $j = 2$ implies

$$Y^T c_2 = \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} \implies \begin{bmatrix} y_1^T c_2 \\ y_2^T c_2 \\ y_3^T c_2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix},$$

i.e., $\langle y_1, c_2 \rangle = -1$, $\langle y_2, c_2 \rangle = 1$, and $\langle y_3, c_2 \rangle = 1$, and similarly for the other c_j .

$Q \subset H$: Let $v \in Q$. Then

$$|\langle v, y_k \rangle| = \left| \langle c_1, y_k \rangle + \sum_{j=1}^3 s_j \langle v_j, y_k \rangle \right| = \left| 1 + \sum_{j=1}^3 s_j \langle v_j, y_k \rangle \right|,$$

whereas

$$\langle v_j, y_k \rangle = \langle c_{j+1} - c_1, y_k \rangle = \begin{cases} 1 - 1, & \text{if } k = j, \\ -1 - 1, & \text{if } k \neq j. \end{cases}$$

Thus, $|\langle v_j, y_k \rangle| = |1 - 2s_k|$, and so $s_k \in [0, 1]$ implies that $1 - 2s_k \in [-1, 0]$, and, hence, $|\langle v_j, y_k \rangle| \leq 1$

$H \subset Q$: Equivalently, we prove the inclusion $Q^c \subset H^c$ of complements. Let $v \notin Q$. First, v_1, v_2, v_3 , are the images of $(-2, 0, 0)^T$, $(0, -2, 0)^T$, $(0, 0, -2)^T$, respectively, under the transformation $(Y^T)^{-1}$. Hence, $\{v_1, v_2, v_3\}$ is a basis for \mathbb{R}^3 . Thus, there are unique elements $s_1, s_2, s_3 \in \mathbb{R}^3$ such that $v - c_1 = s_1 v_1 + s_2 v_2 + s_3 v_3$, i.e.,

$$v = c_1 + s_1 v_1 + s_2 v_2 + s_3 v_3.$$

Because of the uniqueness of the s_j 's, $v \notin Q$ implies there is a $j_0 \in \{1, 2, 3\}$ such that $s_{j_0} \notin [0, 1]$. Now, $|\langle v, y_{j_0} \rangle| = |1 - 2s_{j_0}|$, and so $s_{j_0} \notin [0, 1]$ implies

$$1 - 2s_{j_0} \in (-\infty, -1) \cup (1, \infty).$$

Thus, $|\langle v, y_{j_0} \rangle| > 1$, and so $v \notin H$. Therefore, we have proven $H \subset Q$.

We complete the proof of Lemma V.2 as follows. For the set $\{b, y_1, y_2, y_3\} \subset S^2$, let

$$|\langle b, y_{k_b} \rangle| = \max \{|\langle b, y_1 \rangle|, |\langle b, y_2 \rangle|, |\langle b, y_3 \rangle|\},$$

and set $\lambda_b = \langle b, y_{k_b} \rangle$. Then, for any $k = 1, 2, 3$,

$$\left| \left\langle \frac{b}{\lambda_b}, y_k \right\rangle \right| = \frac{|\langle b, y_k \rangle|}{|\langle b, y_{k_b} \rangle|} \leq \frac{|\langle b, y_{k_b} \rangle|}{|\langle b, y_{k_b} \rangle|} = 1,$$

and so $\frac{b}{\lambda_b} \in Q$. Now $v \in C$ implies that the elements of $\{|\langle v, y_k \rangle| : k = 1, 2, 3\}$ are all equal. By the contrapositive of this implication, we see that the assumption that the elements of $\{|\langle b, y_k \rangle| : k = 1, 2, 3\}$ are not all equal implies $\frac{b}{\lambda_b} \notin C$. Thus, we have shown $\frac{b}{\lambda_b} \in Q \setminus C$. Therefore, by Lemma V.1, we have $\left\| \frac{b}{\lambda_b} \right\| < \|c\|$; and, hence, $b \in S^2$ implies

$$\frac{1}{|\lambda_b|} = \frac{1}{|\lambda_b|} \|b\| = \left\| \frac{b}{\lambda_b} \right\| < \|c\|.$$

We conclude that

$$\begin{aligned} \max \{|\langle b, y_k \rangle| : k = 1, 2, 3\} &= |\lambda_b| \\ &> \frac{1}{\|c\|} = \max \left\{ \left| \left\langle \frac{c}{\|c\|}, y_k \right\rangle \right| : k = 1, 2, 3 \right\}, \end{aligned}$$

and so Lemma V.2 is proved. Q.E.D.

We can now prove the following theorem.

Theorem V.3 ((4,3)-Grassmannian). Let $U = \{u_1, u_2, u_3, u_4\} \subset S^2 \subset \mathbb{R}^3$. If U is (4,3)-Grassmannian,

then U is equiangular, i.e., $|\langle u_k, u_l \rangle| = \beta \in [0, 1]$ whenever $k \neq l$.

Proof: We show the contrapositive of the above implication, viz., we prove that if U is not equiangular, then there is a 4 element set $X \subset S^2$ such that

$$\mathcal{M}_\infty(X) < \mathcal{M}_\infty(U).$$

Hence, U does not have minimal maximum correlation, and therefore it is not $(4, 3)$ -Grassmannian.

Suppose $U = \{u_1, u_2, u_3, u_4\}$ is not equiangular. Then there is an $m_1 \in \{1, 2, 3, 4\}$ such that, if k_1, k_2, k_3 are the remaining indices, we have

$$\max \{|\langle u_{m_1}, u_{k_1} \rangle|, |\langle u_{m_1}, u_{k_2} \rangle|, |\langle u_{m_1}, u_{k_3} \rangle|\} = \mathcal{M}_\infty(U)$$

and

$$|\langle u_{m_1}, u_{k_1} \rangle|, |\langle u_{m_1}, u_{k_2} \rangle|, |\langle u_{m_1}, u_{k_3} \rangle| \text{ are not all equal.}$$

Applying Lemma V.2 with $b = u_{m_1}$ and $\{y_1, y_2, y_3\} = \{u_{k_1}, u_{k_2}, u_{k_3}\}$, there is $c \in \mathbb{R}^3$ such that

$$\begin{aligned} & \max \{|\langle u_{m_1}, u_{k_i} \rangle| : i = 1, 2, 3, \} \\ & > \max \left\{ \left| \left\langle \frac{c}{\|c\|}, u_{k_i} \right\rangle \right| : i = 1, 2, 3, \right\}. \end{aligned}$$

Let $x_{m_1} = \frac{c}{\|c\|}$, see step 2 in Figure 4. Since we have only moved the point u_{m_1} to x_{m_1} , the remaining correlations are unaffected since they do not involve u_{m_1} . Thus

$$\begin{aligned} \mathcal{M}_\infty(U) &= \max \{|\langle u_{m_1}, u_{k_i} \rangle| : i = 1, 2, 3, \} \\ &> \max \{|\langle x_{m_1}, u_{k_i} \rangle| : i = 1, 2, 3, \} =: \alpha. \end{aligned} \quad (\text{V.3})$$

Now either $\mathcal{M}_\infty(\{x_{m_1}, u_{k_1}, u_{k_2}, u_{k_3}\}) = \alpha$, or there is an $m_2 \in \{1, 2, 3, 4\} \setminus \{m_1\}$ such that if m_1, j_1, j_2 are the remaining indices, then

$$\mathcal{M}_\infty(U) = \max \{|\langle u_{m_2}, u_{j_1} \rangle|, |\langle u_{m_2}, u_{j_2} \rangle|\} \quad (\text{V.4})$$

and

$$|\langle u_{m_2}, x_{m_1} \rangle|, |\langle u_{m_2}, u_{j_1} \rangle|, |\langle u_{m_2}, u_{j_2} \rangle| \text{ are not all equal,} \quad (\text{V.5})$$

where (V.5) follows from (V.3). In this case we apply Lemma V.2 to $b = u_{m_2}$ and $\{y_1, y_2, y_3\} = \{u_{j_1}, u_{j_2}, x_{m_1}\}$. Thus, there is a $c' \in \mathbb{R}^3$ such that

$$\begin{aligned} & \max \{|\langle u_{m_2}, x_{m_1} \rangle|, |\langle u_{m_2}, u_{j_1} \rangle|, |\langle u_{m_2}, u_{j_2} \rangle|\} \\ &= \max \{|\langle u_{m_2}, u_{j_1} \rangle|, |\langle u_{m_2}, u_{j_2} \rangle|\} \\ &> \max \left\{ \left| \left\langle \frac{c'}{\|c'\|}, x_{m_1} \right\rangle \right|, \left| \left\langle \frac{c'}{\|c'\|}, u_{j_1} \right\rangle \right|, \left| \left\langle \frac{c'}{\|c'\|}, u_{j_2} \right\rangle \right| \right\}. \end{aligned}$$

Let $x_{m_2} = \frac{c'}{\|c'\|}$, see step 3 in Figure 4. Thus

$$\begin{aligned} \mathcal{M}_\infty(U) &= \max \{|\langle u_{m_2}, u_{j_1} \rangle|, |\langle u_{m_2}, u_{j_2} \rangle|\} \\ &> \max \{|\langle x_{m_2}, x_{m_1} \rangle|, |\langle x_{m_2}, u_{j_1} \rangle|, |\langle x_{m_2}, u_{j_2} \rangle|\} \\ &=: \alpha'. \end{aligned} \quad (\text{V.6})$$

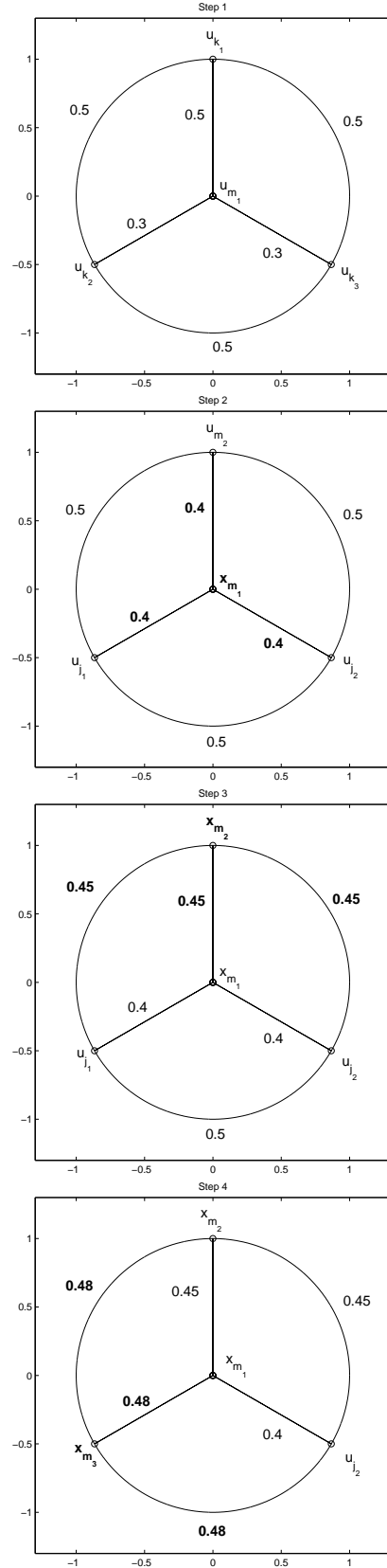


Fig. 4. An example of the four steps in proving Theorem V.3. A number next to an edge represents the inner product of the two boundary points of the edge.

Therefore, (V.3) and (V.6) imply

$$\begin{aligned} & \mathcal{M}_\infty(U) \\ & > \max \left\{ \begin{array}{l} |\langle x_{m_1}, u_{j_1} \rangle|, |\langle x_{m_1}, u_{j_2} \rangle|, \\ |\langle x_{m_2}, x_{m_1} \rangle|, |\langle x_{m_2}, u_{j_1} \rangle|, \\ |\langle x_{m_2}, u_{j_2} \rangle| \end{array} \right\} \\ & = \max \{ \alpha, \alpha' \}, \end{aligned} \quad (\text{V.7})$$

because $j_1, j_2 \in \{k_1, k_2, k_3\}$.

So either $\mathcal{M}_\infty(\{x_{m_1}, x_{m_2}, u_{j_1}, u_{j_2}\}) = \max \{ \alpha, \alpha' \}$ or else $\mathcal{M}_\infty(U) = |\langle u_{j_1}, u_{j_2} \rangle|$.

In the latter case, (V.6) implies that $|\langle u_{j_1}, u_{j_2} \rangle|, |\langle u_{j_1}, x_{m_1} \rangle|, |\langle u_{j_1}, x_{m_2} \rangle|$ are not all equal, and so we apply Lemma V.2 to $b = u_{j_1}$, and $\{y_1, y_2, y_3\} = \{u_{j_2}, x_{m_1}, x_{m_2}\}$. Thus, there is $c'' \in \mathbb{R}^3$ such that

$$\begin{aligned} & \max \{ |\langle u_{j_1}, x_{m_1} \rangle|, |\langle u_{j_1}, x_{m_2} \rangle|, |\langle u_{j_1}, u_{j_2} \rangle| \} \\ & = |\langle u_{j_2}, u_{j_1} \rangle| \\ & > \max \left\{ \begin{array}{l} \left| \left\langle \frac{c''}{\|c''\|}, x_{m_1} \right\rangle \right|, \left| \left\langle \frac{c''}{\|c''\|}, x_{m_2} \right\rangle \right|, \\ \left| \left\langle \frac{c''}{\|c''\|}, u_{j_2} \right\rangle \right| \end{array} \right\}. \end{aligned} \quad (\text{V.8})$$

Let $x_{m_3} = \frac{c''}{\|c''\|}$ and let $X = \{x_{m_1}, x_{m_2}, x_{m_3}, u_{j_2}\}$. Then (V.7) and (V.8) imply

$$\begin{aligned} & \mathcal{M}_\infty(U) \\ & > \max \left\{ \begin{array}{l} |\langle x_{m_3}, x_{m_1} \rangle|, |\langle x_{m_3}, x_{m_2} \rangle|, |\langle x_{m_3}, u_{j_2} \rangle|, \\ |\langle x_{m_2}, x_{m_1} \rangle|, |\langle x_{m_2}, u_{j_2} \rangle|, |\langle x_{m_1}, u_{j_2} \rangle| \end{array} \right\} \\ & = \mathcal{M}_\infty(X). \end{aligned} \quad (\text{V.9})$$

Q.E.D.

Next we show that if a four element set is equiangular then the vectors are parallel to the diagonals of a cube or to four of the diagonals of an icosahedron.

Theorem V.4. *If $u_1, u_2, u_3, u_4 \in S^2$ and $|\langle u_k, u_l \rangle| = \alpha$ for $k, l \in \{1, \dots, 4\}$ with $k \neq l$, then*

$$\alpha = \frac{1}{3} \text{ or } \alpha = \frac{1}{\sqrt{5}}$$

Proof: Since sign changes and rotations do not effect inner products, let P be an element of SO_3 which rotates u_1 to $\delta_3 = (1, 0, 0)^T$. For $k = 1, 2, 3, 4$, let

$$\varepsilon_k = \text{sign} \langle Px_k, \delta_3 \rangle,$$

and let $Q \in SO_3$ so that Q fixes δ_3 and Q rotates $\varepsilon_k Px_2$ to the positive xz -plane, i.e., $\langle Q\varepsilon_k Px_2, \delta_1 \rangle \geq 0$ and $\langle Q\varepsilon_k Px_2, \delta_2 \rangle = 0$. Then, for $k \neq l$,

$$\alpha = |\langle u_k, u_l \rangle| = |\langle \varepsilon_k QP u_k, \varepsilon_l QP u_l \rangle| = |\langle w_k, w_l \rangle|,$$

where $w_k = \varepsilon_k QP u_k$. By the choice of ε_k , for $k = 2, 3, 4$, we have

$$\alpha = |\langle w_1, w_k \rangle| = \langle \delta_3, w_k \rangle,$$

so that the third component of w_k is α . Also, $0 = \langle \delta_2, w_2 \rangle$, and $w_2 \in S^2$, so that the first component of w_2 is $\sqrt{1 - \alpha^2}$.

	$\langle w_2, w_3 \rangle$	$\langle w_2, w_4 \rangle$	$\langle w_3, w_4 \rangle$	
case 1	α	α	α	impossible
case 2	$-\alpha$	α	α	$\alpha = 1/\sqrt{5}$
case 3	$-\alpha$	$-\alpha$	α	$\alpha = 1/\sqrt{5}$
case 4	$-\alpha$	$-\alpha$	$-\alpha$	$\alpha = 1/3$

TABLE III

FOUR MAIN CASES IN THE PROOF OF THEOREM V.4.

Therefore, we have

$$\begin{aligned} w_1 &= (0, 0, 1)^T \\ w_2 &= (\sqrt{1 - \alpha^2}, 0, \alpha)^T \\ w_3 &= (x_3, y_3, \alpha)^T \\ w_4 &= (x_4, y_4, \alpha)^T. \end{aligned} \quad (\text{V.10})$$

We now have four cases (see Table III) where both case 2 and 3 have three subcases which, by relabeling, can be reduced to the considered case.

Case 1. For $k = 3, 4$, $\langle w_2, w_k \rangle = \alpha$ implies

$$x_k = \frac{\alpha - \alpha^2}{\sqrt{1 - \alpha^2}} = \alpha \sqrt{\frac{1 - \alpha}{1 + \alpha}}. \quad (\text{V.11})$$

Then (V.11) and $\|w_k\|^2 = 1$ imply

$$y_k = \pm \sqrt{\frac{1 + \alpha - 2\alpha^2}{1 + \alpha}}. \quad (\text{V.12})$$

In addition, (V.11) and $\langle w_3, w_4 \rangle = \alpha$ imply

$$y_3 \cdot y_4 = \frac{\alpha(1 - \alpha)}{1 + \alpha}. \quad (\text{V.13})$$

Combining (V.12) and (V.13), we have

$$\begin{aligned} -\frac{1 + \alpha - 2\alpha^2}{1 + \alpha} &= \frac{\alpha(1 - \alpha)}{1 + \alpha} \implies 2\alpha^2 + 1 = 0 \\ &\implies \alpha \in \mathbb{C} \setminus \mathbb{R}; \end{aligned}$$

hence, case 1 is impossible.

Case 2. Now $\langle w_2, w_3 \rangle = \alpha$ implies

$$x_3 = \frac{\alpha - \alpha^2}{\sqrt{1 - \alpha^2}}, \quad (\text{V.14})$$

and $\langle w_2, w_4 \rangle = -\alpha$ implies

$$x_4 = \frac{-\alpha - \alpha^2}{\sqrt{1 - \alpha^2}}, \quad (\text{V.15})$$

and (V.14), and (V.15) imply

$$y_3 \cdot y_4 = \alpha. \quad (\text{V.16})$$

Then, (V.14) and $\|w_3\|^2 = 1$ imply

$$y_3^2 = -\frac{2\alpha^2 - \alpha - 1}{\alpha + 1} = \frac{(2\alpha + 1)(\alpha - 1)}{\alpha + 1}, \quad (\text{V.17})$$

and (V.15) and $\|w_4\|^2 = 1$ imply

$$y_4^2 = \frac{2\alpha^2 + \alpha - 1}{\alpha - 1} = \frac{(2\alpha - 1)(\alpha + 1)}{\alpha - 1}. \quad (\text{V.18})$$

Finally, (V.16), (V.17), and (V.18) imply

$$-\alpha^2 = (2\alpha + 1)(2\alpha - 1) \implies \alpha = \pm \frac{1}{\sqrt{5}}.$$

Since α is assumed to be positive, we have proven case 2.

Case 3. For $k = 3, 4$, $\langle w_2, w_k \rangle = -\alpha$ implies

$$x_k = \frac{-\alpha - \alpha^2}{\sqrt{1 - \alpha^2}} = -\alpha \sqrt{\frac{1 + \alpha}{1 - \alpha}}. \quad (\text{V.19})$$

Then (V.19) and $\|w_k\|^2 = 1$ imply

$$y_k^2 = \frac{2\alpha^2 + \alpha - 1}{\alpha - 1} = \frac{(2\alpha - 1)(\alpha + 1)}{\alpha - 1}. \quad (\text{V.20})$$

Hence, (V.19) and $\langle w_3, w_4 \rangle = \alpha$ imply

$$y_3 \cdot y_4 = \frac{\alpha - 3\alpha^2}{1 - \alpha}. \quad (\text{V.21})$$

Combining (V.20) and (V.21), we have

$$\begin{aligned} -\frac{(2\alpha - 1)(\alpha + 1)}{\alpha - 1} = -y_k^2 = y_3 \cdot y_4 = \frac{\alpha - 3\alpha^2}{1 - \alpha} \\ \implies \alpha = \pm \frac{1}{\sqrt{5}}, \end{aligned}$$

and since α is positive, we have proven case 3.

Case 4. This is the same as case 3 except that $\langle w_3, w_4 \rangle = \alpha$ and (V.19) imply

$$y_3 \cdot y_4 = \frac{\alpha(\alpha + 1)}{\alpha - 1}. \quad (\text{V.22})$$

Combining (V.20) and (V.22), we have

$$\begin{aligned} -\frac{(2\alpha - 1)(\alpha + 1)}{\alpha - 1} = -y_k^2 = y_3 \cdot y_4 = \frac{\alpha(\alpha + 1)}{\alpha - 1} \\ \implies \alpha = \frac{1}{3}, \end{aligned}$$

and we have proven case 4.

Therefore, the theorem is proved. Q.E.D.

By Theorem V.4, and since $\frac{1}{\sqrt{5}} > \frac{1}{3}$, we see that the $(4, 3)$ -Grassmannian bound is $\frac{1}{3}$. which is also seen to be optimal by inspection.

VI. $(5, 3)$ -GRASSMANNIAN FRAMES

We first introduce some ideas from convex analysis, [17], [18], [19].

Definition VI.1. A set $A \subset \mathbb{R}^n$ is *convex* if for any $x_1, x_2 \in A$, and for any $\lambda \in [0, 1]$,

$$\lambda x_1 + (1 - \lambda)x_2 \in A.$$

A point $x \in A$ is an *extreme point* of A if whenever $x = \lambda x_1 + (1 - \lambda)x_2$, where $0 < \lambda < 1$ and $x_1, x_2 \in A$, then $x = x_1 = x_2$. Given a set $A \subset \mathbb{R}^n$, the *convex hull* of A is

Hull(A)

$$= \left\{ \sum_{j=1}^m \lambda_j x_j : \sum_{j=1}^m \lambda_j = 1, \lambda_j > 0, x_j \in A, m \in \mathbb{N} \right\}.$$

There is the following relationship between extreme points, convex hulls, and convex sets, [20].

Theorem VI.2. A nonempty bounded convex set in \mathbb{R}^d is the convex hull of its set of extreme points.

We need the following two convexity propositions to prove Lemma VI.5, which in turn is used to prove Lemma VI.6, the key lemma for computing the $(5, 3)$ -Grassmannian bound in Theorem VI.7.

Proposition VI.3. Let $N \geq d$, let $Y = \{y_1, \dots, y_N\} \subset S^{d-1} \subset \mathbb{R}^d$, and assume $\text{span}(Y) = \mathbb{R}^d$. Let

$$Q = \{v \in \mathbb{R}^d : |\langle v, y_k \rangle| \leq 1, \text{ for } k = 1, \dots, N\}$$

and let C be the set of extreme points of Q . Then

- Q is a bounded convex set,
- If $v_0 \in C$ then there are at least d distinct integers $k_1, \dots, k_d \in \{1, \dots, N\}$ such that $|\langle v_0, y_{k_i} \rangle| = 1$ for $i = 1, \dots, d$,
- $\text{card}(C) \leq \binom{N}{d} 2^d < \infty$.

Under the same hypotheses of Proposition VI.3 we have the following result, whose proof is in Appendix C.

Proposition VI.4. Let N, d, Y, Q , and C be as in Proposition VI.3, and let $c \in C$ have the property that $\|c\| = \max\{\|c'\| : c' \in C\}$. Then, for any $v \in Q \setminus C$,

$$\|v\| < \|c\|.$$

Following the basic geometric idea in [10], we can reduce the correlation of a given frame. The following lemma requires the previous propositions as well as Theorem IV.2.

Lemma VI.5. Let $U = \{b, y_1, y_2, y_3, y_4\} \subset S^2 \subset \mathbb{R}^3$, and let $\alpha = \mathcal{M}_\infty(U)$. Assume $|\langle b, y_1 \rangle| < \alpha$ and $|\langle b, y_2 \rangle| < \alpha$. Then there exists $c \in \mathbb{R}^3$ such that

$$\left| \left\langle \frac{c}{\|c\|}, y_k \right\rangle \right| < \alpha \text{ for } k = 1, 2, 3, 4.$$

Lemma VI.6. Let $U = \{u_1, \dots, u_5\}$ be a $(5, 3)$ -Grassmannian frame, and let $\alpha = \mathcal{M}_\infty(U)$. Then for any j , there are distinct $j_1, j_2, j_3 \in \{1, \dots, 5\} \setminus \{j\}$ such that

$$|\langle u_j, u_{j_k} \rangle| = \alpha \text{ for } k = 1, 2, 3.$$

Proof: We prove the contrapositive. By relabeling if necessary, without loss of generality, assume $|\langle u_1, u_2 \rangle| < \alpha$ and $|\langle u_1, u_3 \rangle| < \alpha$. We use Lemma VI.5 to construct a new set W for which $\mathcal{M}_\infty(W) < \alpha$. This shows U is not $(5, 3)$ -Grassmannian.

First, let $b = u_1$ and $\{y_1, \dots, y_4\} = \{u_2, \dots, u_5\}$ and apply Lemma VI.5. Then there is a $c_1 \in \mathbb{R}^3$ such that

$$\left| \left\langle \frac{c_1}{\|c_1\|}, u_k \right\rangle \right| < \alpha \text{ for } k = 2, 3, 4, 5.$$

Second, consider the set $\tilde{U} := \{u_2, \dots, u_5\}$. We have two cases,

Case 1. There exist $j_0, k_0 \in \{2, 3, 4, 5\}$ with $j_0 \neq k_0$, for which $|\langle u_{j_0}, u_{k_0} \rangle| < \alpha$.

For ease in notation, by relabeling if necessary, we assume $j_0 = 2$ and $k_0 = 3$. In this case, we can apply Lemma

VI.5 with $b = u_2$ and $\{y_1, \dots, y_4\} = \left\{ \frac{c_1}{\|c_1\|}, u_3, u_4, u_5 \right\}$, and construct $c_2 \in \mathbb{R}^3$ such that

$$\left| \left\langle \frac{c_1}{\|c_1\|}, \frac{c_2}{\|c_2\|} \right\rangle \right| < \alpha$$

and

$$\max \left\{ \left| \left\langle \frac{c_2}{\|c_2\|}, u_k \right\rangle \right| : k = 3, 4, 5 \right\} < \alpha.$$

Now we can apply Lemma VI.5 to the remaining points and produce a frame with a strictly smaller value of \mathcal{M}_∞ . In fact, since $\left| \left\langle \frac{c_i}{\|c_i\|}, u_3 \right\rangle \right| < \alpha$ for $i = 1, 2$, we let $b = u_3$ and $\{y_1, \dots, y_4\} = \left\{ \frac{c_1}{\|c_1\|}, \frac{c_2}{\|c_2\|}, u_4, u_5 \right\}$. Then, by Lemma VI.5, there is a $c_3 \in \mathbb{R}^d$ such that

$$\left| \left\langle \frac{c_3}{\|c_3\|}, \frac{c_i}{\|c_i\|} \right\rangle \right| < \alpha \quad \text{for } i = 1, 2,$$

and

$$\max \left\{ \left| \left\langle \frac{c_3}{\|c_3\|}, u_k \right\rangle \right| : k = 4, 5 \right\} < \alpha.$$

Finally, apply Lemma VI.5 one last time to $b = u_4$ and

$$\{y_1, \dots, y_4\} = \left\{ \frac{c_1}{\|c_1\|}, \frac{c_2}{\|c_2\|}, \frac{c_3}{\|c_3\|}, u_5 \right\},$$

and obtain $c_4 \in \mathbb{R}^d$ for which

$$\left| \left\langle \frac{c_4}{\|c_4\|}, \frac{c_i}{\|c_i\|} \right\rangle \right| < \alpha \quad \text{for } i = 1, 2, 3,$$

and

$$\left| \left\langle \frac{c_4}{\|c_4\|}, u_5 \right\rangle \right| < \alpha.$$

Thus, if we let $W = \left\{ \frac{c_1}{\|c_1\|}, \frac{c_2}{\|c_2\|}, \frac{c_3}{\|c_3\|}, \frac{c_4}{\|c_4\|}, u_5 \right\}$, then, by construction, for any $i, j \in \{1, \dots, 4\}$, $i \neq j$, we have $\left| \left\langle \frac{c_i}{\|c_i\|}, \frac{c_j}{\|c_j\|} \right\rangle \right| < \alpha$ and $\left| \left\langle \frac{c_i}{\|c_i\|}, u_5 \right\rangle \right| < \alpha$. Hence,

$$\mathcal{M}_\infty(W) < \alpha = \mathcal{M}_\infty(U),$$

and so U is not $(5, 3)$ -Grassmannian. This finishes Case 1.

Case 2. \tilde{U} is equiangular.

Since \tilde{U} has four elements, Theorem V.4 implies $\alpha = 1/3$ or $\alpha = 1/\sqrt{5}$. If $\alpha = 1/3$, then set

$$\beta = \max \left\{ \left| \left\langle \frac{c_1}{\|c_1\|}, u_k \right\rangle \right| : k = 2, 3, 4, 5 \right\}.$$

Thus, by construction of c_1 , we have $\beta < \frac{1}{3}$ and

$$\mathcal{M}_\infty \left(\left\{ \frac{c_1}{\|c_1\|} \right\} \cup \tilde{U} \right) = \max \left\{ \frac{1}{3}, \beta \right\} = \frac{1}{3},$$

whereas Theorem IV.2 with $N = 5$ and $d = 3$ implies

$$\frac{1}{\sqrt{6}} \leq \mathcal{M}_\infty \left(\left\{ \frac{c_1}{\|c_1\|} \right\} \cup \tilde{U} \right) = \frac{1}{3},$$

a contradiction.

Thus, $\alpha = \frac{1}{\sqrt{5}}$; and $|\langle u_1, u_k \rangle| < \alpha$ for $k = 2, 3, 4, 5$, and $|\langle u_k, u_j \rangle| = \alpha$ for $k \neq j$ and $k, j \in \{2, 3, 4, 5\}$.

We seek to find a contradiction. Without loss of generality, the setting can reduce to the following general position by using rotations and sign changes as in Theorem V.4:

$$\begin{aligned} u_2 &= (0, 0, 1)^T \\ u_3 &= (\sqrt{1-\alpha^2}, 0, \alpha)^T \\ u_4, u_5 &\in \{p_1, p_2, p_3, p_4\}, \end{aligned}$$

where

$$\begin{aligned} p_1 &= \left(\alpha \sqrt{\frac{1-\alpha}{1+\alpha}}, \sqrt{\frac{(1+2\alpha)(1-\alpha)}{1+\alpha}}, \alpha \right)^T \\ &= \left(\sqrt{1-\alpha^2} \cos\left(\frac{2\pi}{5}\right), \sqrt{1-\alpha^2} \sin\left(\frac{2\pi}{5}\right), \alpha \right)^T, \end{aligned}$$

$$\begin{aligned} p_2 &= \left(-\alpha \sqrt{\frac{1+\alpha}{1-\alpha}}, \sqrt{\frac{(1-2\alpha)(1+\alpha)}{1-\alpha}}, \alpha \right)^T \\ &= \left(\sqrt{1-\alpha^2} \cos\left(\frac{4\pi}{5}\right), \sqrt{1-\alpha^2} \sin\left(\frac{4\pi}{5}\right), \alpha \right)^T, \end{aligned}$$

$$\begin{aligned} p_3 &= \left(-\alpha \sqrt{\frac{1+\alpha}{1-\alpha}}, -\sqrt{\frac{(1-2\alpha)(1+\alpha)}{1-\alpha}}, \alpha \right)^T \\ &= \left(\sqrt{1-\alpha^2} \cos\left(-\frac{4\pi}{5}\right), \sqrt{1-\alpha^2} \sin\left(-\frac{4\pi}{5}\right), \alpha \right)^T, \end{aligned}$$

and

$$\begin{aligned} p_4 &= \left(\alpha \sqrt{\frac{1-\alpha}{1+\alpha}}, -\sqrt{\frac{(1+2\alpha)(1-\alpha)}{1+\alpha}}, \alpha \right)^T \\ &= \left(\sqrt{1-\alpha^2} \cos\left(-\frac{2\pi}{5}\right), \sqrt{1-\alpha^2} \sin\left(-\frac{2\pi}{5}\right), \alpha \right)^T. \end{aligned}$$

Therefore, if

$$A = \begin{pmatrix} \cos(2\pi/5) & -\sin(2\pi/5) & 0 \\ \sin(2\pi/5) & \cos(2\pi/5) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and $p_0 = u_3$, then

$$A^k(p_0, p_1, p_2, p_3, p_4) = (p_{\sigma(0)}, p_{\sigma(1)}, p_{\sigma(2)}, p_{\sigma(3)}, p_{\sigma(4)}),$$

where $\sigma(n) = (n+k) \pmod{5}$.

If we set $\beta = |\langle u_1, u_2 \rangle| < \alpha$, then, by changing the sign of u_1 if necessary and since $\|u_1\| = 1$, we may assume

$$u_1 = \left(\sqrt{1-\beta^2} \cos t_0, \sqrt{1-\beta^2} \sin t_0, \beta \right)^T,$$

for some fixed $t_0 \in [-\pi, \pi)$. Hence,

$$\begin{aligned} |\langle u_1, u_3 \rangle| &< \alpha & \text{(VI.1)} \\ \iff \left| \sqrt{1-\alpha^2} \sqrt{1-\beta^2} \cos t_0 + \alpha\beta \right| &< \alpha \\ \iff \frac{-\alpha}{\sqrt{1-\alpha^2}} \frac{1+\beta}{\sqrt{1-\beta^2}} < \cos t_0 < \frac{\alpha}{\sqrt{1-\alpha^2}} \frac{1-\beta}{\sqrt{1-\beta^2}} \\ \iff \underbrace{\cos^{-1}\left(\frac{1}{2} \sqrt{\frac{1-\beta}{1+\beta}}\right)}_{\gamma_1(\beta)} < |t_0| < \underbrace{\cos^{-1}\left(-\frac{1}{2} \sqrt{\frac{1+\beta}{1-\beta}}\right)}_{\gamma_2(\beta)}. & \text{(VI.2)} \end{aligned}$$

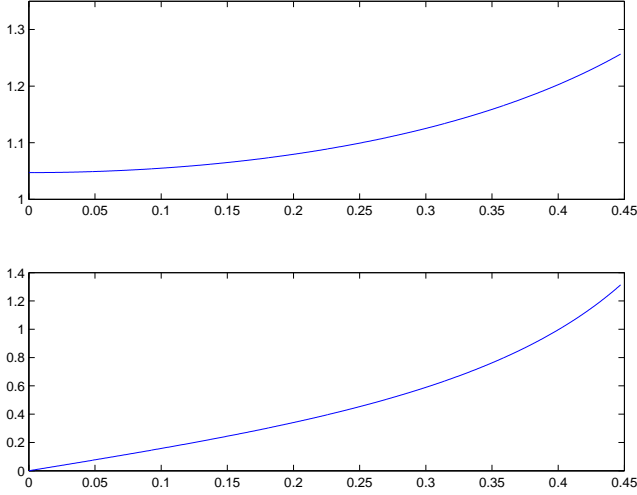


Fig. 5. Top figure is the function $\gamma_2 - \gamma_1$, bottom figure is the function $\frac{d}{d\beta}(\gamma_2 - \gamma_1)$. We can see that the original function is strictly increasing.

We observe that

$$\gamma_1(\beta) = \begin{cases} \frac{6\pi}{15} = \frac{2\pi}{5}, & \text{if } \beta = \alpha, \\ \frac{5\pi}{15} = \frac{\pi}{3}, & \text{if } \beta = 0, \end{cases}$$

$$\gamma_2(\beta) = \begin{cases} \frac{12\pi}{15} = \frac{4\pi}{5}, & \text{if } \beta = \alpha, \\ \frac{10\pi}{15} = \frac{2\pi}{3}, & \text{if } \beta = 0, \end{cases}$$

and that $\frac{d}{d\beta}(\gamma_2 - \gamma_1)(\beta) > 0$ for $\beta \in (0, \alpha)$, see Figure 5. Thus $\frac{5\pi}{15} \leq \gamma_2(\beta) - \gamma_1(\beta) < \frac{6\pi}{15}$, when $\beta \in [0, \alpha)$.

Hence, for a fixed $\beta \in [0, \alpha)$,

$$\gamma_2(\beta) < \gamma_1(\beta) + \frac{6\pi}{15},$$

and, for $k = 1, 2, 3, 4$, we have

$$\begin{aligned} \alpha &> |\langle u_1, p_k \rangle| = |\langle A^{-k}u_1, A^{-k}p_k \rangle| \\ &= |\langle A^{-k}u_1, p_0 \rangle| = |\langle A^{-k}u_1, u_3 \rangle|, \end{aligned}$$

where

$$\begin{aligned} A^{-k}u_1 &= \left(\sqrt{1 - \beta^2} \cos\left(t_0 - \frac{2\pi k}{5}\right), \right. \\ &\quad \left. \sqrt{1 - \beta^2} \sin\left(t_0 - \frac{2\pi k}{5}\right), \beta \right)^T. \end{aligned}$$

Therefore, by (VI.2),

$$\alpha > |\langle u_1, p_k \rangle| \iff \gamma_1(\beta) \leq \left| t_0 - \frac{2\pi k}{5} \right| \leq \gamma_2(\beta), \quad (\text{VI.3})$$

for $k = 0, 1, 2, 3, 4$. These inequalities define ten intervals on the torus $\mathbb{T}_{2\pi}$. If we plot these ten intervals in Figure 6, we note that no set of three of them overlap, see Figure 6. This

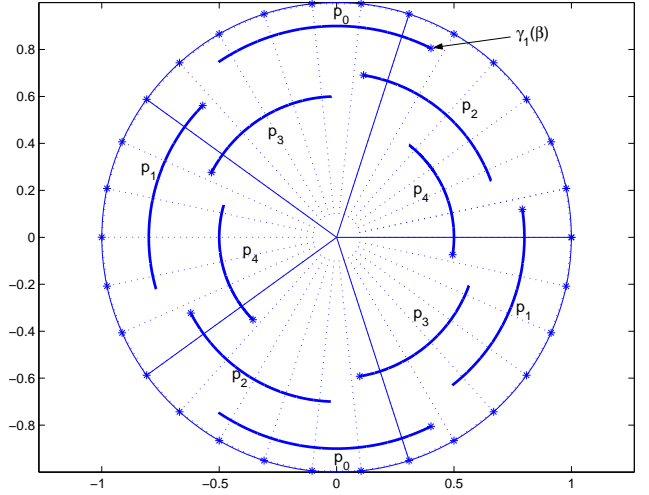


Fig. 6. Ten intervals on $\mathbb{T}_{2\pi}$ corresponding to the points $p_0 = u_3$, and p_1, \dots, p_4 .

assertion can also be seen since

$$\begin{aligned} \gamma_1(\beta) &\leq \left| t_0 - \frac{2\pi k}{5} \right| \leq \gamma_2(\beta) \\ \implies \gamma_1(\beta) &\leq \left| t_0 - \frac{2\pi k}{5} \right| < \gamma_1(\beta) + \frac{2\pi}{5} \\ \implies t_0 &\in \underbrace{[\gamma + \varepsilon k, \gamma + \varepsilon(k+1)]}_{P_k} \\ &\quad \cup \underbrace{[-\gamma + \varepsilon(k-1), -\gamma + \varepsilon k]}_{N_k} \end{aligned}$$

where $\gamma = \gamma_1(\beta)$, $\varepsilon = \frac{2\pi}{5}$, and $k = 0, 1, 2, 3, 4$. Thus, $\cup_{k=0}^4 P_k$ is a disjoint cover of $\mathbb{T}_{2\pi} \setminus [\gamma - \varepsilon, \gamma)$, and $\cup_{k=0}^4 N_k$ is a disjoint cover of $\mathbb{T}_{2\pi} \setminus [-\gamma + \varepsilon, -\gamma)$. Hence, t_0 can be in at most two of the ten sets P_k, N_k .

Now by assumption, $|\langle u_1, u_3 \rangle| = |\langle u_1, p_0 \rangle| < \alpha$. Also $|\langle u_1, u_4 \rangle| < \alpha$, and $|\langle u_1, u_5 \rangle| < \alpha$ where $u_4, u_5 \in \{p_1, p_2, p_3, p_4\}$. Thus, (VI.3) implies t_0 lies in three of the ten intervals represented in Figure 6, a contradiction. Consequently, \tilde{U} cannot be equiangular. Q.E.D.

Finally, using Lemma VI.6, we have the following result.

Theorem VI.7. *If $U \subset S^2 \subset \mathbb{R}^3$ is $(5, 3)$ -Grassmannian, then $\mathcal{M}_\infty(U) = \frac{1}{\sqrt{5}}$.*

Proof: Let $\alpha = \mathcal{M}_\infty(U)$, and consider the graph whose vertices are u_1, \dots, u_5 , and whose edges are defined as follows: for any pair of points $u_k, u_j \in U$ with $k \neq j$, an edge connects u_k and u_j if and only if $|\langle u_k, u_j \rangle| = \alpha$. We call the number of edges emanating from a vertex u_k , the *degree* of u_k , denoted $\deg(u_k)$. Then Lemma VI.6 implies that

$$\sum_{k=1}^5 \deg(u_k) \geq \sum_{k=1}^5 3 = 15.$$

Since each edge connects two vertices, the sum of the degrees must be an even number. Thus, at least one vertex u_j must have degree 4, i.e., there is a $j \in \{1, \dots, 5\}$, such that

$|\langle u_j, u_{j_i} \rangle| = \alpha$ for $i = 1, \dots, 4$, where $\{j_1, j_2, j_3, j_4\} = \{1, 2, 3, 4, 5\} \setminus \{j\}$. By relabeling if necessary we may assume

$$|\langle u_1, u_k \rangle| = \alpha \text{ for } k = 2, 3, 4, 5,$$

and

$$|\langle u_2, u_k \rangle| = \alpha \text{ for } k = 3, 4.$$

Furthermore, we can reduce to the general position used in Theorem V.4, i.e., assume

$$\begin{aligned} u_1 &= (0, 0, 1)^T \\ u_2 &= (\sqrt{1 - \alpha^2}, 0, \alpha)^T \\ u_3 &= (x_3, y_3, \alpha)^T \\ u_4 &= (x_4, y_4, \alpha)^T \\ u_5 &= (x_5, y_5, \alpha)^T. \end{aligned}$$

We have two cases.

Case 1. $|\langle u_3, u_4 \rangle| = \alpha$.

Then the subset $U = \{u_1, u_2, u_3, u_4\}$ is equiangular, hence Theorem V.4 implies $\alpha = \frac{1}{3}$ or $\frac{1}{\sqrt{5}}$. However, just as in Lemma VI.6, $\alpha = \frac{1}{3}$ implies that

$$\frac{1}{3} = \mathcal{M}_\infty(U) \leq \frac{1}{\sqrt{6}},$$

and so $\alpha = \frac{1}{\sqrt{5}}$.

Case 2. $|\langle u_3, u_4 \rangle| < \alpha$.

Then since each vertex must be of degree 3, we have that $|\langle u_3, u_5 \rangle|$ and $|\langle u_4, u_5 \rangle|$ each equals α . Thus, if we remove the absolute values, we have the following equations:

$$\begin{aligned} \langle u_2, u_3 \rangle &= \pm\alpha, & \langle u_2, u_4 \rangle &= \pm\alpha, \\ \langle u_3, u_5 \rangle &= \pm\alpha, & \langle u_4, u_5 \rangle &= \pm\alpha. \end{aligned}$$

This gives $2^4 = 16$ possible cases. Of these 16 cases, 7 lead to contradictions, and the remaining 9 fall into 5 types; but each implies that u_3, u_4, u_5 are three of the four points

$$\begin{aligned} &\left(\alpha \sqrt{\frac{1 - \alpha}{1 + \alpha}}, \pm \sqrt{\frac{(1 + 2\alpha)(1 - \alpha)}{1 + \alpha}}, \alpha \right)^T, \\ &\left(-\alpha \sqrt{\frac{1 + \alpha}{1 - \alpha}}, \pm \sqrt{\frac{(1 - 2\alpha)(1 + \alpha)}{1 - \alpha}}, \alpha \right)^T, \end{aligned}$$

which are the positive endpoints on the remaining 4 diagonals of an icosahedron. Hence in each case, $\alpha = 1/\sqrt{5}$. Q.E.D.

The (5, 3)-Grassmannian frame is the first example of a non-optimal Grassmannian frame since $\frac{1}{\sqrt{5}} > \frac{1}{\sqrt{6}}$. Hence, by Theorem IV.2, the (5, 3)-Grassmannian frame is the first three dimensional example of a Grassmannian frame which is not tight.

VII. (6, 3)-GRASSMANNIAN FRAMES

The (6, 3)-Grassmannian bound can be calculated as a consequence of Theorem IV.2.

Theorem VII.1. *If $U = \{u_1, \dots, u_6\} \subset S^2$ is (6, 3)-Grassmannian, then*

$$\mathcal{M}_\infty(U) = 1/\sqrt{5}.$$

Proof: Set $\alpha = \frac{1}{\sqrt{5}}$, and consider the set W with vertices

$$\begin{aligned} w_1 &= (0, 0, 1)^T, \\ w_2 &= \left(\sqrt{1 - \alpha^2}, 0, \alpha \right)^T, \\ w_3 &= \left(\alpha \sqrt{\frac{1 - \alpha}{1 + \alpha}}, \sqrt{\frac{(1 + 2\alpha)(1 - \alpha)}{1 + \alpha}}, \alpha \right)^T, \\ w_4 &= \left(\alpha \sqrt{\frac{1 - \alpha}{1 + \alpha}}, -\sqrt{\frac{(1 + 2\alpha)(1 - \alpha)}{1 + \alpha}}, \alpha \right)^T, \\ w_5 &= \left(-\alpha \sqrt{\frac{1 + \alpha}{1 - \alpha}}, \sqrt{\frac{(1 - 2\alpha)(1 + \alpha)}{1 - \alpha}}, \alpha \right)^T, \\ w_6 &= \left(-\alpha \sqrt{\frac{1 + \alpha}{1 - \alpha}}, -\sqrt{\frac{(1 - 2\alpha)(1 + \alpha)}{1 - \alpha}}, \alpha \right)^T. \end{aligned}$$

Note that $\pm W$ are the twelve vertices of an icosahedron. For $k \neq l$, we compute $|\langle w_k, w_l \rangle| = \frac{1}{\sqrt{5}}$. Furthermore, by Theorem IV.2, if U is a 6 element subset of S^2 , then

$$\mathcal{M}_\infty(U) \geq \sqrt{\frac{6 - 3}{3(6 - 1)}} = \frac{1}{\sqrt{5}} = \mathcal{M}_\infty(W).$$

Thus W is a (6, 3)-Grassmannian frame. Q.E.D.

Notice the (6, 3) Grassmannian arrangement is so good that when one removes a vector from it, it remains Grassmannian, and when one removes two vectors from it, it is still a local minimum of \mathcal{M}_∞ . In [4] Conway, Hardin, and Sloane have found that there are other instances of this in higher dimensions, particularly when the symmetry group of the frame has a large number of elements.

APPENDIX A

We show that Grassmannian frames exist. First, we define the function

$$\begin{aligned} f &: \underbrace{S^{d-1} \times \dots \times S^{d-1}}_{N \text{ times}} \rightarrow [0, 1] \\ f(x_1, \dots, x_N) &= \mathcal{M}_\infty(\{x_k\}_{k=1}^N). \end{aligned}$$

Next we check that f is continuous on $X := \mathbb{R}^d \times \dots \times \mathbb{R}^d$ (N times). Consider the norm on X defined by

$$\left\| \{x_k\}_{k=1}^N \right\|_X = \sum_{k=1}^N \|x_k\|,$$

let $\{x_k\}_{k=1}^N \in X$ be fixed, set $R - 1 = \max_k \{\|x_k\|\}$, and let $\varepsilon > 0$ be given. Clearly $R \geq 1$. Choose δ such that $0 < \delta < \frac{\sqrt{1 + \varepsilon} - 1}{R}$, i.e., $R^2 \delta^2 + 2R\delta < \varepsilon$. Then, whenever $\left\| \{y_k\}_{k=1}^N - \{x_k\}_{k=1}^N \right\|_X < \delta$, we have that, for every $j \in \{1, \dots, N\}$,

$$\|y_j - x_j\| \leq \sum_{k=1}^N \|y_k - x_k\| = \left\| \{y_k\}_{k=1}^N - \{x_k\}_{k=1}^N \right\|_X < \delta.$$

Therefore, for each j , there is an $\alpha_j \in \mathbb{R}^d$ with $\|\alpha_j\| < \delta$ such that $y_j = x_j + \alpha_j$. Thus,

$$\begin{aligned} & |f(y_1, \dots, y_N) - f(x_1, \dots, x_N)| \\ &= \max_{k \neq l} \{ |\langle x_k, x_l \rangle| + |\langle x_k, \alpha_l \rangle| + |\langle \alpha_k, x_l \rangle| + |\langle \alpha_k, \alpha_l \rangle| \} \\ &\quad - \max_{k \neq l} \{ |\langle x_k, x_l \rangle| \} \\ &\leq \max_{k \neq l} \{ |\langle x_k, x_l \rangle| + \|x_k\| \|\alpha_l\| + \|\alpha_k\| \|x_l\| + \|\alpha_k\| \|\alpha_l\| \} \\ &\quad - \max_{k \neq l} \{ |\langle x_k, x_l \rangle| \} \\ &< \max_{k \neq l} \{ |\langle x_k, x_l \rangle| \} + 2R\delta + R\delta^2 - \max_{k \neq l} \{ |\langle x_k, x_l \rangle| \} \\ &= 2R\delta + R\delta^2 < \varepsilon. \end{aligned}$$

Hence, f is continuous on the compact set $S^{d-1} \times \dots \times S^{d-1}$ (N times), and so f achieves its absolute maximum and absolute minimum on this set. Thus, we know that (N, d) -Grassmannian frames exist for any $N \geq d$. Next we must check that if U_d^N solves (I.2), then U_d^N is a unit norm frame for \mathbb{R}^d , but this a tautology since, by compactness, U_d^N is one of the frames over which we are taking the infimum.

APPENDIX B

Proof: [Proof of Lemma IV.1]

We proceed by induction. Let $P(n)$ be the statement

$$\det(H_n) = (1 + (n-1)\beta)(1-\beta)^{n-1}$$

and

$$\det(C_n) = \beta(1-\beta)^{n-1}.$$

For $n = 1$, $H_1 = 1$ and $C_1 = \beta$, and so $\det(H_1) = 1$ and $\det(C_1) = \beta$; this is $P(1)$.

Next assume $P(n)$. Using the cofactor expansion of the determinant, we first note that the $(1, 1)$ -cofactor of H_{n+1} and C_{n+1} is $\det(H_n)$. Also note that for $j = 2, \dots, n+1$, the $(1, j)$ -cofactor of both H_{n+1} and C_{n+1} is

$$(-1)^{1+j} \det(B_n^{(j)}),$$

where $B_n^{(j)}$ can be defined recursively as

$$\begin{aligned} B_n^{(1)} &= C_n, \\ B_n^{(j)} &= \tilde{B}_n^{(j-1)} \quad \text{for } j = 2, \dots, n+1, \end{aligned}$$

and where $\tilde{B}_n^{(j-1)}$ is $B_n^{(j-1)}$ with the j th and $(j-1)$ st rows interchanged. Since \det is multilinear, interchanging a row changes the sign of the determinant. Hence

$$(-1)^{1+j} \det(B_n^{(j)}) = -\det(C_n) \quad \text{for } j = 2, \dots, n+1.$$

Using the induction hypothesis and the cofactor expansion, we compute

$$\begin{aligned} \det(H_{n+1}) &= 1 \cdot \det(H_n) + \sum_{j=2}^{n+1} \left(\beta \cdot (-1)^{1+j} \det(B_n^{(j)}) \right) \\ &= \det(H_n) - n\beta \det(C_n) \\ &= (1 + (n-1)\beta)(1-\beta)^{n-1} - n\beta^2(1-\beta)^{n-1} \\ &= (1 + n\beta)(1-\beta)(1-\beta)^{n-1} \end{aligned}$$

and

$$\begin{aligned} \det(C_{n+1}) &= \beta \det(H_n) - n\beta \det(C_n) \\ &= \beta(1 + (n-1)\beta)(1-\beta)^{n-1} - n\beta^2(1-\beta)^{n-1} \\ &= (\beta - \beta^2)(1-\beta)^{n-1}; \end{aligned}$$

this is $P(n+1)$, and so the result follows by induction. Q.E.D.

Proof: [Proof of Theorem IV.2]

a. First, we prove the inequality (IV.3). Since the $N \times N$ Gramian matrix G is symmetric, the spectral theorem applies, and so G has N eigenvalues λ_j counted with multiplicity and ordered by size, i.e., $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N$. Furthermore, since $\text{rank}(G) = d_0$, only the first d_0 of these eigenvalues are nonzero. Hence,

$$\sum_{k=1}^{d_0} \lambda_k = \text{Trace } G = \sum_{k=1}^N |\langle x_k, x_k \rangle| = \sum_{k=1}^N 1 = N.$$

Now set $e_k = \lambda_k - \frac{N}{d_0}$. Then

$$\sum_{k=1}^{d_0} e_k = \sum_{k=1}^{d_0} \left(\lambda_k - \frac{N}{d_0} \right) = N - d_0 \frac{N}{d_0} = 0,$$

and so

$$\begin{aligned} \sum_{k=1}^{d_0} \lambda_k^2 &= \sum_{k=1}^{d_0} \left(\frac{N}{d_0} + e_k \right)^2 \\ &= \sum_{k=1}^{d_0} \frac{N^2}{d_0^2} + \frac{2N}{d_0} \sum_{k=1}^{d_0} e_k + \sum_{k=1}^{d_0} e_k^2 \\ &= \frac{N^2}{d_0} + \sum_{k=1}^{d_0} e_k^2 \geq \frac{N^2}{d_0}, \end{aligned}$$

with equality if and only if $e_k = 0$ for $k = 1, \dots, d_0$, i.e., if and only if $\lambda_k = \frac{N}{d_0}$ for $k = 1, \dots, d_0$. Next, the eigenvalues of G^2 are $\lambda_1^2 \geq \lambda_2^2 \geq \dots \geq \lambda_N^2$, so that if g_k is the k th column of G , then by matrix multiplication we have

$$\begin{aligned} \frac{N^2}{d_0} &\leq \sum_{k=1}^{d_0} \lambda_k^2 = \text{Trace}(G^2) = \sum_{k=1}^N g_k^T g_k \quad (\text{B.1}) \\ &= \sum_{k=1}^N \sum_{l=1}^N |\langle x_k, x_l \rangle|^2. \end{aligned}$$

Since G is symmetric, $|\langle x_k, x_l \rangle| = |\langle x_l, x_k \rangle|$, so that by B.1 we compute

$$\begin{aligned} \frac{N^2}{d_0} &\leq \sum_{k=1}^N \sum_{l=1}^N |\langle x_k, x_l \rangle|^2 \\ &= \sum_{k=l} |\langle x_k, x_l \rangle|^2 + \sum_{k < l} |\langle x_k, x_l \rangle|^2 + \sum_{k > l} |\langle x_k, x_l \rangle|^2 \\ &= N + 2 \sum_{k < l} |\langle x_k, x_l \rangle|^2 \\ &\leq N + 2 \frac{N(N-1)}{2} \max_{k \neq l} \{ |\langle x_k, x_l \rangle|^2 \}. \end{aligned} \quad (\text{B.2})$$

Therefore, solving for the max in (B.2), we have

$$\frac{N - d_0}{d_0(N - 1)} \leq \mathcal{M}_\infty (X_d^N)^2. \quad (\text{B.3})$$

For future reference we note that $d \geq d_0$ implies $\frac{N-d}{d(N-1)} \leq \frac{N-d_0}{d_0(N-1)}$. Hence, (IV.3) remain true when we replace d with $d_0 \leq d$.

b. Next we prove that equality holds in (IV.3) if and only if X_d^N is equiangular and is a tight frame for its span.

(\implies): Suppose $\mathcal{M}_\infty(X_d^N) = \sqrt{\frac{N-d_0}{d_0(N-1)}}$. Then (B.2) becomes

$$\sum_{k=1}^N \sum_{l=1}^N |\langle x_k, x_l \rangle|^2 = \frac{N^2}{d_0},$$

which implies from (B.1) that

$$\sum_{k=1}^{d_0} \lambda_k^2 = \frac{N^2}{d_0};$$

and, as we saw above, equality in this sum implies that $\lambda_k = \frac{N}{d_0}$ for $k = 1, \dots, d_0$. The frame bounds for X_d^N are the largest and smallest nonzero eigenvalues, and hence $A = N/d_0 = B$ and so X_d^N is a tight frame for its span.

To see that X_d^N is also equiangular, we notice that (B.2) gives

$$N + 2 \sum_{k < l} |\langle x_k, x_l \rangle|^2 = \frac{N^2}{d_0},$$

and, hence,

$$\sum_{k < l} |\langle x_k, x_l \rangle|^2 = \frac{N(N - d_0)}{2d_0}. \quad (\text{B.4})$$

Our assumption $\max_{k \neq l} |\langle x_k, x_l \rangle|^2 = \frac{N-d_0}{d_0(N-1)}$ implies that, for any $k \neq l$,

$$|\langle x_k, x_l \rangle|^2 = \frac{N - d_0}{d_0(N - 1)} - \varepsilon_{k,l},$$

where $\varepsilon_{k,l} \geq 0$. Thus (B.4) is

$$\begin{aligned} \frac{N(N - d_0)}{2d_0} &= \sum_{k < l} \left(\frac{N - d_0}{d_0(N - 1)} - \varepsilon_{k,l} \right) \\ &= \left(\frac{N(N - 1)}{2} \right) \left(\frac{N - d_0}{d_0(N - 1)} \right) - \sum_{k < l} \varepsilon_{k,l} \\ &= \frac{N(N - d_0)}{2d_0} - \sum_{k < l} \varepsilon_{k,l}. \end{aligned}$$

Therefore, $\sum_{k < l} \varepsilon_{k,l} = 0$, and, since the $\varepsilon_{k,l}$ are non-negative, we can assert that $\varepsilon_{k,l} = 0$ for $k < l$. Also, since G is symmetric, $\varepsilon_{k,l} = 0$ for all $k \neq l$, and hence X_d^N is equiangular with $|\langle x_k, x_l \rangle|^2 = \frac{N-d_0}{d_0(N-1)}$.

(\Leftarrow): Now assume X_d^N is equiangular and is a tight frame for its span with frame bound $A = B = \frac{N}{d_0}$. Then there is an $\alpha \in [0, 1]$, such that $|\langle x_k, x_l \rangle|^2 = \alpha$ for $k \neq l$. Now since X_d^N is tight, $\lambda_k = \frac{N}{d_0}$ for $k = 1, \dots, d_0$, and zero otherwise. Hence (B.1) and (B.2) imply

$$\frac{N^2}{d_0} = \sum_{k=1}^{d_0} \lambda_k^2 = \sum_{k=1}^N \sum_{l=1}^N |\langle x_k, x_l \rangle|^2 = N + N(N - 1)\alpha.$$

Thus, solving for α we see that equality holds in (IV.3).

c. Finally, to prove $N > \frac{d(d+1)}{2}$ implies X_d^N is not equiangular, we prove the contrapositive using Lemma IV.1 and the following argument, cf., [21]. Assume X_d^N is equiangular. Let $P_k : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be the projection of x onto the line spanned by x_k , i.e., $P_k x = \langle x, x_k \rangle x_k$. Let V be the vector space of symmetric linear mappings $\mathbb{R}^d \rightarrow \mathbb{R}^d$. Then $\dim(V) = \frac{d(d+1)}{2}$, and the map $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{R}$ given by $\langle C, D \rangle = \text{Trace}(CD)$ is an inner product on V . Since X_d^N is equiangular, there is an $\alpha \in [0, 1]$ such that $\langle x_k, x_l \rangle = \pm\alpha$ for $k \neq l$. Furthermore, $\alpha = 1$ implies $N = 2$, since the elements of X_d^N are assumed to be distinct and of unit norm. Thus, for $d \geq 2$, we have $N = 2 < 3 \leq \frac{d(d+1)}{2}$. Therefore, we may assume $\alpha \in [0, 1)$. Now,

$$\langle P_k, P_l \rangle = \langle x_k, x_l \rangle^2 = \begin{cases} 1, & \text{if } k = l \\ \alpha^2, & \text{if } k \neq l. \end{cases}$$

Hence, the Gramian of the set $\{P_1, \dots, P_N\} \subset V$ is

$$[G]_{k,l} = [\langle P_k, P_l \rangle]_{k,l} = \begin{cases} 1, & \text{if } k = l \\ \alpha^2, & \text{if } k \neq l, \end{cases}$$

where $[G]_{k,l}$ is the (k, l) th entry of the matrix G . Thus, Lemma IV.1 applies with $G = H_N$ and $\beta = \alpha^2$. Consequently, if $\alpha \in [0, 1)$, then

$$\det G = (1 + (N - 1)\alpha^2) (1 - \alpha^2)^{N-1} \neq 0.$$

Therefore, G is invertible and has full rank. Finally, since $\text{rank}(G) = \text{rank}(S) = N$, we have that

$$\begin{aligned} N = \text{rank}(G) &= \dim(\text{span}\{P_1, \dots, P_N\}) \\ &\leq \dim(V) = \frac{d(d+1)}{2}. \end{aligned}$$

We have proved that if X_d^N is equiangular, then $N \leq d(d+1)/2$; and so, by contraposition, we have proven the result. Q.E.D.

APPENDIX C

Proof: [Proof of Proposition VI.4]

Let $v \in Q \setminus C$. Then there is a $\lambda \in (0, 1)$, and there are $x_1, x_2 \in Q$ with $x_1 \neq x_2$ such that $v = \lambda x_1 + (1 - \lambda)x_2$. Consider the function $f : \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$f(\lambda) = \|\lambda x_1 + (1 - \lambda)x_2\|.$$

We first verify that f is uniformly continuous on \mathbb{R} . Let $\varepsilon > 0$ be given, and choose $\delta < \frac{\varepsilon}{\|x_1 - x_2\|}$. Then, for all λ_0 for which $|\lambda - \lambda_0| < \delta$, we have

$$\begin{aligned} |f(\lambda) - f(\lambda_0)| &= \left| \|\lambda x_1 + (1 - \lambda)x_2\| - \|\lambda_0 x_1 + (1 - \lambda_0)x_2\| \right| \\ &\leq \|\lambda x_1 + (1 - \lambda)x_2 - \lambda_0 x_1 - (1 - \lambda_0)x_2\| \\ &= \|(\lambda - \lambda_0)(x_1 - x_2)\| \\ &= |\lambda - \lambda_0| \|x_1 - x_2\| \\ &< \delta \|x_1 - x_2\| < \varepsilon. \end{aligned}$$

Now set $g(\lambda) = f(\lambda)^2$. Then $g(\lambda)$ is also continuous on \mathbb{R} and it is the parabola,

$$\begin{aligned} g(\lambda) &= \|\lambda x_1 + (1 - \lambda)x_2\|^2 \\ &= \lambda^2 \|x_1\|^2 + 2(\lambda - \lambda^2) \langle x_1, x_2 \rangle - 2(1 - \lambda) \|x_2\|^2. \end{aligned}$$

We compute

$$g'(\lambda) = 2\lambda \|x_1 - x_2\|^2 + 2 \langle x_1 - x_2, x_2 \rangle,$$

so that $g'(\lambda) = 0$ at

$$\lambda_* = -\frac{\langle x_1 - x_2, x_2 \rangle}{\|x_1 - x_2\|^2}.$$

Furthermore, for all $\lambda \in \mathbb{R}$,

$$g''(\lambda) = 2\|x_1 - x_2\|^2 > 0. \quad (\text{C.1})$$

Hence, g attains a minimum at λ_* , and for all $\lambda \neq \lambda_*$, we have $g(\lambda) > g(\lambda_*)$. Now if we restrict g to $[0, 1]$, then g achieves its maximum and minimum on $[0, 1]$. Thus, if $\lambda_* \in [0, 1]$, then by (C.1) and the fact that g describes a parabola, we have

$$\min_{\lambda \in [0, 1]} g(\lambda) = g(\lambda_*)$$

and

$$\max_{\lambda \in [0, 1]} g(\lambda) = \max \{g(0), g(1)\};$$

and if $\lambda_* \notin [0, 1]$, then

$$\min_{\lambda \in [0, 1]} g(\lambda) = \min \{g(0), g(1)\}$$

and

$$\max_{\lambda \in [0, 1]} g(\lambda) = \max \{g(0), g(1)\}.$$

In either case the maximum of g occurs at one of the end points. Furthermore, at interior points, g is strictly less than the maximum value.

Now since $\|v\|^2 = g(\lambda_0)$ for some $\lambda_0 \in (0, 1)$, (C.1) implies

$$\begin{aligned} \|v\|^2 &= g(\lambda_0) \\ &< \max_{\lambda \in [0, 1]} g(\lambda) = \max \{g(0), g(1)\} = \max \left\{ \|x_1\|^2, \|x_2\|^2 \right\}. \end{aligned}$$

Thus, we have shown that

$$v \in Q \setminus C \implies \exists x \in Q \text{ such that } \|v\| < \|x\|$$

and, hence,

$$v \in Q \setminus C \implies \|v\| < \sup \{\|x\| : x \in Q\}. \quad (\text{C.2})$$

Q is a bounded closed set so that, by continuity of $\|\cdot\|$, the supremum in (C.2) is achieved on Q , whereas (C.2) also shows that this supremum is not achieved on $Q \setminus C$. Thus,

$$\sup \{\|x\| : x \in Q\} = \sup \{\|x\| : x \in C\} = \|c\|.$$

Therefore, for any $v \in Q \setminus C$ we have $\|v\| < \sup \{\|x\| : x \in Q\} = \|c\|$. Q.E.D.

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