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NEARLY ORTHOGONAL VECTORS AND SMALL ANTIPODAL SPHERICAL CODES

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ABSTRACT. How can $d+k$ vectors in $\mathbb{R}^d$ be arranged so that they are as close to orthogonal as possible? In particular, define $\theta(d,k) := \min_X \max_{x\neq y\in X} |\langle x,y\rangle|$ where the minimum is taken over all collections of $d+k$ unit vectors $X \subseteq \mathbb{R}^d$. In this work, we focus on the case where k is fixed and $d\to\infty$. In establishing bounds on $\theta(d,k)$, we find an intimate connection to the existence of systems of $\binom{k+1}{2}$ equiangular lines in $\mathbb{R}^k$. Using this connection, we are able to pin down $\theta(d,k)$ whenever $k\in\{1,2,3,7,23\}$ and establish asymptotics for general k. The main tool is an upper bound on $\mathbb{E}_{x,y\sim\mu}|\langle x,y\rangle|$ whenever μ is an isotropic probability mass on $\mathbb{R}^k$, which may be of independent interest. Our results translate naturally to the analogous question in $\mathbb{C}^d$. In this case, the question relates to the existence of systems of k^2 equiangular lines in $\mathbb{C}^k$, also known as SIC-POVM in physics literature.

How can a given number of points be arranged on a sphere in $\mathbb{R}^d$ so that they are as far from each other as possible? This is a basic problem in coding theory; for example, the book [**5**] is devoted to this problem exclusively. Such point arrangements are called *spherical codes.* Most constructions of spherical codes are symmetric. Here we consider the *antipodal codes*, in which the points come in pairs $x,-x$. In other words, we seek arrangements of $d+k$ unit vectors in $\mathbb{R}^d$ so that they are as close to orthogonal as possible. An alternative point of view is that these are codes in the projective space $\mathbb{RP}^{d-1}$; for example, see [**2**]. We focus on the case when k is small.

As we will see, this question relates to the problem of the existence of large families of equiangular lines in $\mathbb{R}^k$. Similarly, the analogous question for unit vectors in $\mathbb{C}^d$ relates to equiangular lines in $\mathbb{C}^k$, which are the mathematical underpinning of symmetric informationally complete measurements in quantum theory [**9**]. Because of this, we elect to treat the real and complex cases in parallel. Henceforth, we denote by $\mathbb{H}$ the underlying field, which can be either $\mathbb{R}$ or $\mathbb{C}$.

For $\mathbb{H}\in\{\mathbb{R},\mathbb{C}\}$, define the parameter

$$\theta_{\mathbb{H}}(d,k) := \min_X \max_{x\neq y\in X} |\langle x,y\rangle|,$$

where the minimum is taken over all collections of $d+k$ unit vectors $X\subseteq\mathbb{H}^d$. In this paper, we prove bounds on $\theta_{\mathbb{H}}(d,k)$ when k is fixed and $d\to\infty$.

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For a collection of vectors $X = \{x_1, \dots, x_n\} \subseteq \mathbb{H}^d$, the *Gram matrix* is the matrix $A \in \mathbb{H}^{n\times n}$ where $A_{ij} = \langle x_i, x_j\rangle$. It will be easier to work with the Gram matrices than with the vectors themselves.

For a matrix $A \in \mathbb{H}^{n\times n}$, define $\operatorname{off}(A) := \max_{i\neq j} |A_{ij}|$. By considering Gram matrices, one can equivalently define $\theta_{\mathbb{H}}(d,k) = \min_A \operatorname{off}(A)$ where the minimum is taken over all $A \in \mathbb{H}^{(d+k)\times(d+k)}$ with $\operatorname{rk}(A) = d$ where $A_{ii} = 1$ for every i and A is Hermitian and positive semidefinite. Our techniques are not specialized to Hermitian, positive semidefinite matrices, so we also define

$$\operatorname{off}_{\mathbb{H}}(d,k) := \min_A \operatorname{off}(A),$$

where the minimum is taken over all $A \in \mathbb{H}^{(d+k)\times(d+k)}$ with $\operatorname{rk}(A) = d$ and $A_{ii} = 1$ for every i. Note that $\operatorname{off}_{\mathbb{H}}(d,k) \le \theta_{\mathbb{H}}(d,k)$.

We show that there is an intimate connection between determining these parameters and the existence of large systems of equiangular lines in $\mathbb{H}^k$.

Definition 1. A system of equiangular lines in $\mathbb{H}^k$ is a collection of unit vectors $X \subseteq \mathbb{H}^k$ so that there is some $\beta \in \mathbb{R}$ where $|\langle x,y\rangle| = \beta$ for all $x \neq y \in X$.

It is known that if $X \subseteq \mathbb{R}^k$ is a system of equiangular lines, then $|X| \le \binom{k+1}{2}$ and if $X \subseteq \mathbb{C}^k$ is a system of equiangular lines, then $|X| \le k^2$.

The main results of this paper are as follows:

Theorem 2.
1. *For positive integers d, k,*

$$\operatorname{off}_{\mathbb{R}}(d,k) \ge \frac{1}{\alpha_k(d+k)-1},$$

where $\alpha_k = \frac{(k-1)\sqrt{k+2}+2}{k(k+1)}$. If equality holds, then there exists a system of $\binom{k+1}{2}$ equiangular lines over $\mathbb{R}^k$ and $d \equiv -k \pmod{\binom{k+1}{2}}$.

2. *For positive integers d, k,*

$$\operatorname{off}_{\mathbb{C}}(d,k) \ge \frac{1}{\alpha^*_k(d+k)-1},$$

where $\alpha^*_k = \frac{(k-1)\sqrt{k+1}+1}{k^2}$. If equality holds, then there exists a system of k^2 equiangular lines over $\mathbb{C}^k$ and $d \equiv -k \pmod{k^2}$.

This is an improvement over the classical Welch bound [**10**] when $k \le O(d^{1/2})$. It is a quantitative improvement of a result of Cohn–Kumar–Minton [**2**, Corollary 2.13] which asserts that Welch bound is not sharp for $k \le O(d^{1/2})$, without providing a better bound.

A computer-assisted proof of the case $(d,k) = (4,2)$ of Theorem 2 was recently given by Fickus–Jasper–Mixon [**6**].

We show also that equality in Theorem 2 does, in fact, hold under the stated conditions.

Theorem 3.

1. *If there is a system of* $\binom{k+1}{2}$ *equiangular lines in* $\mathbb{R}^k$ *and* $d \equiv -k \pmod{\binom{k+1}{2}}$*, then*
$$\mathrm{off}_{\mathbb{R}}(d,k) = \theta_{\mathbb{R}}(d,k) = \frac{1}{\alpha_k(d+k)-1},$$
where $\alpha_k = \frac{(k-1)\sqrt{k+2}+2}{k(k+1)}$.
2. *If there is a system of* k^2 *equiangular lines in* $\mathbb{C}^k$ *and* $d \equiv -k \pmod{k^2}$*, then*
$$\mathrm{off}_{\mathbb{C}}(d,k) = \theta_{\mathbb{C}}(d,k) = \frac{1}{\alpha_k^*(d+k)-1},$$
where $\alpha_k^* = \frac{(k-1)\sqrt{k+1}+1}{k^2}$.

The usual way of proving bounds on codes is to use linear programming. In the context of spherical codes, the relevant linear program first appeared in the work of Delsarte, Goethals and Seidel [**3**]. See [**5**, Chapter 2] for the general exposition, and [**1**] for the case of few vectors.

In contrast, we establish Theorem 2 by relating the problem to that of bounding the first moment of isotropic measures.

Definition 4. For $\mathbb{H} \in \{\mathbb{R}, \mathbb{C}\}$, a probability mass μ on $\mathbb{H}^k$ is called *isotropic* if $\mathbb{E}_{x\sim\mu} |\langle x, v\rangle|^2 = \frac{1}{k}\|v\|^2$ for every $v \in \mathbb{H}^k$. Equivalently, μ is isotropic if $\mathbb{E}_{x\sim\mu} xx^* = \frac{1}{k} I_k$. Such a probability mass is also called a *probabilistic tight frame* with frame constant $1/k$ (see [**4**] for a survey).

We show the following:

Lemma 5.

1. *If* μ *is an isotropic probability mass on* $\mathbb{R}^k$*, then*
$$\mathbb{E}_{x,y\sim\mu} |\langle x, y\rangle| \le \frac{(k-1)\sqrt{k+2}+2}{k(k+1)},$$
with equality if and only if there exists $X \subseteq \mathbb{R}^k$*, a system of* $\binom{k+1}{2}$ *equiangular lines, and* μ *satisfies* $\mu(x) + \mu(-x) = 1/\binom{k+1}{2}$ *for every* $x \in X$.
2. *If* μ *is an isotropic probability mass on* $\mathbb{C}^k$*, then*
$$\mathbb{E}_{x,y\sim\mu} |\langle x, y\rangle| \le \frac{(k-1)\sqrt{k+1}+1}{k^2},$$
with equality if and only if there exists $X \subseteq \mathbb{C}^k$*, a system of* k^2 *equiangular lines, and* μ *satisfies* $\mu(x) + \mu(-x) = 1/k^2$ *for every* $x \in X$.

As there are systems of $\binom{k+1}{2}$ equiangular lines over $\mathbb{R}^k$ whenever $k \in \{1, 2, 3, 7, 23\}$, we can give tight answers for infinitely many d in these cases. See [**7, 8, 11**] for the known bounds of the size of the largest system of equiangular lines in $\mathbb{R}^k$.

Even in the cases not covered by Theorem 3, we still show that Theorem 2 is asymptotically tight.

Theorem 6. *Let $\mathbb{H} \in \{\mathbb{R}, \mathbb{C}\}$. For every $\epsilon > 0$, there is an integer k_0 so that for any fixed $k \geq k_0$,*

$$\theta_{\mathbb{H}}(d,k) \leq \big(1+o(1)\big)\frac{(1+\epsilon)\sqrt{k}}{d},$$

where $o(1) \to 0$ as $d \to \infty$.

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