ABSTRACT

Title of dissertation: SPHERICAL TWO-DISTANCE SETS AND RELATED TOPICS IN HARMONIC ANALYSIS

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This dissertation is devoted to the study of applications of harmonic analysis. The maximum size of spherical few-distance sets had been studied by Delsarte at al. in the 1970s. In particular, the maximum size of spherical two-distance sets in $\mathbb{R}^n$ had been known for $n \leq 39$ except $n = 23$ by linear programming methods in 2008. Our contribution is to extend the known results of the maximum size of spherical two-distance sets in $\mathbb{R}^n$ when $n = 23, 40 \leq n \leq 93$ and $n \neq 46, 78$. The maximum size of equiangular lines in $\mathbb{R}^n$ had been known for all $n \leq 23$ except $n = 14, 16, 17, 18, 19$ and 20 since 1973. We use the semidefinite programming method to find the maximum size for equiangular line sets in $\mathbb{R}^n$ when $24 \leq n \leq 41$ and $n = 43$.

We suggest a method of constructing spherical two-distance sets that also form tight frames. We derive new structural properties of the Gram matrix of a two-distance set that also forms a tight frame for $\mathbb{R}^n$. One of the main results in this part is a new correspondence between two-distance tight frames and certain strongly regular graphs. This allows us to use spectral properties of strongly regular graphs to construct two-distance tight frames. Several new examples are obtained using this characterization.

Bannai, Okuda, and Tagami proved that a tight spherical designs of harmonic index 4 exists if and only if there exists an equiangular line set with the angle $\arccos(1/(2k-1))$ in the Euclidean space of dimension $3(2k-1)^2 - 4$ for each integer $k \geq 2$. We show nonexistence of tight spherical designs of harmonic index 4 on S^{n-1} with $n \geq 3$ by a modification of the semidefinite programming method. We also derive new relative bounds for equiangular line sets. These new relative bounds are usually tighter than previous relative bounds by Lemmens and Seidel.

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by

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Dedication

To my parents, my loving wife, Mei-Chun, my son, Terrence and my daughter Marim.

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Chapter 1
Introduction

1.1 Spherical codes and designs

A spherical code is a finite collection X of unit vectors in $\mathbb{R}^n$. We denote the unit sphere in $\mathbb{R}^n$ by S^{n-1}. The study of spherical codes has been the focus of much interest with an interplay of methods from many aspects of mathematics, physics, and computer science [33]. There are several interesting problems on spherical codes, for instance the sphere packing problem which asks to find out how densely a large number of identical spheres can be packed together, the kissing number problem which seeks to find the maximum number of unit spheres that can touch a unit sphere without overlapping and many other related topics.

The history of sphere packing problems can be traced to Kepler (1610) who conjectured that the maximum density of a sphere packing in $\mathbb{R}^3$ is $\frac{\pi}{\sqrt{18}} \simeq 0.7405$. For $\mathbb{R}^2$, the standard hexagonal packing is optimal with the density $\frac{\pi}{\sqrt{12}} \simeq 0.9079$. In 1998, Hales proved the Kepler conjecture by extensive computer calculation in [47]. The optimal packing is the "face-centered cubic" packing (equivalently, the A_3 or D_3 root lattice). For $\mathbb{R}^n$, where $n \geq 4$, the problem remains unsolved and the bounds are discussed in [53], [33], [31].

The kissing number $k(n)$ has been known only for $n = 1, 2, 3, 4, 8, 24$. Its determination for $n = 1, 2$ is trivial, but it is not the case for other values of n. The case $n = 3$ was the subject of a discussion between Isaac Newton and David Gregory in 1694. Gregory asserted that 13 spheres could be placed in contact with a central sphere and Newton claimed that only 12 were possible. The answer was given 12 by K. Schütte and B. L. van der Waerden [74] in 1953. O. Musin used the variation of linear programming method to prove $k(4) = 24$ [65]. E. Bannai and N .J. A. Sloane solved the case for $n = 8$ and 24 [7]. For other dimensions, $k(n)$ remains open and the bounds are concerned in [5], [64].

Classical results in harmonic analysis imply some nontrivial positive constraints on the point sets of S^{n-1}. We start with the group representation theory. Assume that G is a compact group, then it has an unique normalized measure μ, the Haar measure, which is invariant under G. Let $L_2(G)$ denote the vector space of complex-valued functions u on G satisfying

$$\int_G |u(g)|^2 d\mu(g) < \infty$$

with the inner product

$$\langle u_1, u_2 \rangle = \int_G u_1(g)\overline{u_2(g)} d\mu(g)$$

By the Peter-Weyl Theorem, the space $L_2(G)$ decomposes into a countable direct sum of mutually orthogonal subspaces V_k^n, where V_k^n affords an irreducible unitary representation of G.

In particular, if G is the special orthogonal group $SO(n)$, i.e. the group of isometries of S^{n-1} with determinant 1. $SO(n)$ induces an unique invariant measure on S^{n-1}. Then, $L_2(S^{n-1})$ decomposes into an infinite direct sum of orthogonal subspaces V_k^n which are usually denoted by $\mathrm{Harm}_k(S^{n-1})$. The elements in $\mathrm{Harm}_k(S^{n-1})$ are called spherical harmonic functions. Let us discuss harmonic functions as follows.

Let $\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots \frac{\partial^2}{\partial x_n^2}$ be the Laplace operator. A polynomial $f(x)$ is *harmonic* if $\Delta f(x) = 0$. Then, $\mathrm{Harm}_k(S^{n-1})$ is the space of a harmonic and homogeneous polynomials of degree k restricted to the sphere S^{n-1}.

Let $h_k^n := \dim \mathrm{Harm}_k(S^{n-1})$. Let $\{f_i^n(x) | 1 \leq i \leq h_k^n\}$ be the orthonormal basis of a Hilbert space $\mathrm{Harm}_k(S^{n-1})$. We have the following addition formula:

$$G_k^n(\langle x, y\rangle) = \sum_{i=1}^{h_k^n} f_i(x) f_i(y),$$

where $G_k^n(t)$ only depends on inner product values t and is called the *zonal spherical function* associated with $\mathrm{Harm}_k(S^{n-1})$ or the *Gegenbauer polynomial*. Hence,

$$\begin{aligned}\sum_{x,y\in X^2} G_k^n(\langle x, y\rangle) &= \sum_{x,y\in X^2} \sum_{i=1}^{h_k^n} f_i(x) f_i(y) \\ &= \sum_{i=1}^{h_k^n} \sum_{x,y\in X^2} f_i(x) f_i(y) \\ &= \sum_{i=1}^{h_t^n} (\sum_{x\in X^2} f_i(x))^2 \geq 0\end{aligned}$$

In short, we have

$$\sum_{x,y\in X^2} G_t^n(\langle x, y\rangle) \geq 0 \tag{1.1}$$

The above statements are classical [1], [2], [54].

Philippe Delsarte in the seventies [35] introduced the linear programming (LP) method which is very powerful method to solve extremal problems. The LP method is based on the positivity of Gegenbauer polynomials (1.1). It was initially developed in the framework of association schemes and then extended to the family of 2-points homogeneous spaces, including the compact real manifolds having the property (see [36] [33, Chapter 9] [53]). Let us recall that a 2-point homogeneous space is a metric space on which a group G acts transitively, leaving the distance d invariant, and such that, for $(x, y) \in X^2$, there exists $g \in G$ such that $(gx, gy) = (x', y')$ if and only if $d(x, y) = d(x', y')$. The Hamming space H_n and the unit sphere S^{n-1} are the core examples of such spaces which play a major role in coding theory.

The applications of this method to the study of codes and designs are numerous: very good upper bounds for the number of elements of a code with given minimal distance can be obtained with this method, including a number of cases where this upper bound is tight and leads to a proof of optimality and uniqueness of certain codes, as well as to the best known asymptotic bounds (see [35], [63], [53], [33, Chapter 9], [59]).

We want to indicate that, geometric proof of (1.1) had been given by Schoenberg [72] in 1942, although his work was not known to researchers in the area discussed until at least the 1990s.

The degree $s(X)$ is the number of values assumed by the inner product between distinct vectors in X; that is

$$s(X) = |I(x)|, \quad I(X) = \{\langle x_i, x_j \rangle; x_i, x_j \in X \text{and } i \neq j\}$$

If $s(X) = s$, such sets are called *spherical s-distance sets*. Estimating the maximum size of spherical s-distance sets is a classical problem in distance geometry that has been studied for several decades.

The first major result for upper bounds was obtained by Delsarte, Goethals, and Seidel [36]. They proved that, irrespective of the actual values of the distances, the following "harmonic" bound holds true:

$$|X| \leq \binom{n+s-1}{n-1} + \binom{n+s-2}{n-1} \tag{1.2}$$

The key ideas of their proof are linear programming method which we introduce in (1.1). They also showed that this bound is tight for dimensions $n = 2, 6, 22$ and $s = 2$ in which cases it is related to sets of equiangular lines in dimension $n+1$. In particular, if $|I(x)| = 2$, we call X a *spherical two-distance set*. If a and b are the two inner product values between distinct elements in a spherical two-distance set, there is an important result by Larman et al. [57] to restrict b as a linear function of a. The explicit statement is the following.

Theorem 1.1 (Larman, Rogers, and Seidel [57]) *Let S be a spherical two-distance in $\mathbb{R}^n$. If $|S| > 2n+3$ and $a > b$, then $b = \frac{ka-1}{k-1}$ for some integer k such that $2 \leq k \leq (1+\sqrt{2n})/2$.*

The condition $|S| > 2n+3$ was improved to $|S| > 2n+1$ by Neumaier [69]. He also gave an example of a two-distance set with cardinality $2n+1$ that violates the integeraity condition of k. This example is obtained from the spherical embedding of the conference graph.

Theorem 1.1 is one of the key theorem which we use to determine exact answers of maximum size of spherical two-distance sets up to dimension $n \leq 94$ except $n = 46$ and 78.

There is an another interesting question in spherical codes: how to find a subset on sphere such that it globally approximates the sphere S^{n-1} very well? There is one very reasonable answer introduce by Delsarte, Goethal and Seidel [36] in 1977. They defined the notion of *spherical t-design* as follows.

Definition 1.1 *Let t be a natural number. A finite subset X of the unit sphere S^{n-1} is called a* spherical t-design *if, for any polynomial $f(x) = f(x_1, x_2, \ldots, x_n)$ of degree at most t, the following equality holds :*

$$\frac{1}{|S^{n-1}|} \int_{S^{n-1}} f(x) d\sigma(x) = \frac{1}{|X|} \sum_{x \in X} f(x). \tag{1.3}$$

An equivalent definition of spherical designs can be given in terms of harmonic polynomials. Let $\text{Harm}_t(\mathbb{R}^n)$ be the set of homogeneous harmonic polynomials of degree t on $\mathbb{R}^n$. Then the set X is a spherical design [36] if

$$\sum_{x \in X} f(x) = 0 \quad \forall f(x) \in \text{Harm}_j(\mathbb{R}^n), 1 \leq j \leq t. \tag{1.4}$$

By the definition, we can see that the union of two spherical designs are still spherical designs. Therefore, we are interested in the minimum cardinality of a spherical design when t and n are given. Delsarte, Goethals, and Seidel [36] proved that the cardinality of a spherical t-design X is bounded below,

$$|X| \geq \binom{n+e-1}{n-1} + \binom{n+e-2}{n-1}, \quad |X| \geq 2\binom{n+e-1}{n-1}$$

for $t = 2e$ and $t = 2e+1$. Again, the technique to obtain this lower bounds is still the linear programming method (1.1). The spherical t-design is called tight if any one of these bound is attained. If X is a tight spherical $2s$-design, it is immediately a maximum spherical s-distance set attaining harmonic bound in (1.2). The bounds on few distance sets of spherical codes can be generalized to other metric spaces. Barg and Musin [16] have improved the bounds on the size few distance sets in the Hamming space, the Johnson space and uniform intersecting families of subsets.

1.2 Semidefinite programming

A semidefinite program (SDP) is an optimization problem of the form

$$\max\{\langle X, C\rangle |\ X \succeq 0,\ \langle X, A_i\rangle = b_i, i = 1, \dots, m\}, \tag{1.5}$$

where X is an $n\times n$ variable matrix, $A_1, \dots, A_m$ and C are given Hermitian matrices, $(b_1, \dots, b_m)$ is a given vector and $\langle X, Y\rangle = \text{trace}\,(Y^*X)$ is the inner product of two matrices. Semidefinite programming is an extension of linear programming that has found a range of applications in combinatorial optimization, control theory, distance geometry, and coding theory. General introduction to semidefinite programming is given, for instance, in [17].

Applications of semidefinite programming in coding theory and distance geometry gained momentum after the pioneering work of Schrijver [73] that derived SDP bounds on codes in the Hamming and Johnson spaces. Schijver's approach was based on the so-called Terwilliger algebra of the association scheme and formed a far-reaching generalization of the work of Delsarte [35]. Elements of the groundwork for SDP bounds in the Hamming space were laid by Dunkl [38], although this connection was also made somewhat later [79]. We refer to [62] for a detailed general survey of the approach via association schemes and further references.

The root of SDP method is from the work of Bochner [19] in more general space, called the two-point homogeneous space which we mention in the beginning of this chapter. SDP bounds for the real sphere were derived by Bachoc and Vallentin [5] in the context of the kissing number problem. One of the main results of [5] is that for any finite set of points $\mathcal{C} \subset S^{n-1}$

$$\sum_{(x,y,z)\in\mathcal{C}^3} S_k^n(x\cdot y, x\cdot z, y\cdot z) \succeq 0 \tag{1.6}$$

The matrices S_k^n play the role of the constraints A_i in the general SDP problem (1.5). Explicit definition of S_k^n can be found in Chapter 2. Positivity constraints (1.6) give rise to a general SDP bound on the cardinality of point sets obtained in [5], where it was used to improve upper bounds on $k(n)$ in small dimensions.

We note that constraints (1.1) arise from the unrestricted action of G on S^{n-1}. Constraints (1.6) are obtained by considering actions that fix three given points on the sphere. We also call this by three-point SDP problems. Further SDP bounds can be obtained by considering zonal matrices that arise from actions that fix any given number of points; however even for two points, actual evaluation of the bounds requires significant computational effort [64].

1.3 Equiangular lines

A spherical two-distance set is a finite collection of unit vectors in $\mathbb{R}^n$ such that the distances between any two distinct vectors assume only two values. Therefore, equiangular line sets can be regarded as special type of spherical two-distance sets. A set of lines in a metric space is called equiangular if the angle between each pair of lines is the same. We are interested in upper bounds on the number of equiangular lines in $\mathbb{R}^n$. In other words, if we have a set of unit vectors $S = \{x_i\}_{i=1}^M$ and there is a constant $c > 0$ such that $|\langle x_i, x_j \rangle| = c$ for all $1 \leq i \neq j \leq M$, what is the maximum cardinality of S? Denote this quantity by $M(n)$. The problem of determining $M(n)$ looks elementary but a general answer has so far proved elusive. The history of this problem started with Hanntjes [48] who found $M(n)$ for $n = 2$ and 3 in 1948. The maximal number of equiangular lines in $\mathbb{R}^2$ is 3: we can take the lines through opposite vertices of a regular hexagon, each at an angle 60 degrees from the other two. The maximum in $\mathbb{R}^3$ is 6: we can take lines through opposite vertices of an icosahedron. Van Lint and Seidel [60] found the largest number of equiangular lines for $4 \leq n \leq 7$. The known bounds on $M(n)$ for small dimensions was known exactly only if $2 \leq n \leq 13; n = 15, 21, 22, 23$ [58]. In Chapter 3, we use the semidefinite programming method to derive some new bounds on $M(n)$. In particular, exact values of $M(n)$ are obtained for $24 \leq n \leq 41$ and for $n = 43$ where previous results gave divergent bounds: we show that $M(n) = 276$ for $24 \leq n \leq 41$ and $M(43) = 344$. These results are established by performing computations with SDP. We also show that $M_{1/5}(n) = 276$ for $23 \leq n \leq 60$. These results resolve a part of the Lemmens-Seidel conjecture and enable us to obtain the results. For $44 \leq n \leq 136$, we also obtain new upper bounds on $M(n)$, improving upon the Gerzon bound, although no new exact values are found in this range. We give a more complete table of the computation results in Table 3.3. Recently (March 2014), we were informed that the upper bounds of equiangular line sets in $\mathbb{R}^{14}$ and $\mathbb{R}^{16}$ have been improved by 1 [45]. Therefore, $M(14) = 28$ or 29 and $M(16) = 40$ or 41.

1.4 Finite two-distance tight frames

Frames were introduced in 1952 by Duffin and Schaeffer [37]. Later, the subject was reinvigorated following a publication of Daubechies, Grossman, and Meyer [34]. Since then, frames have been used extensively in signal/image processing where they are called *Gabor frames* or *Weyl-Heisenberg frames* [26], [39], [46], [51]. Many new applications of tight frames have arisen in internet coding [28] [43] [42] [44], wireless communication [49], [76]. Each new application requires a new class of tight frames. After the introduction of *frame potentials* by Benedetto and Fickus [18], there was an explosion of new results concerning the construction of tight frames for finite dimensional Hilbert space [29]. The importance of [18] is that it gives a geometric interpretation for equal-norm finite tight frames along the lines of Coulomb's law in Physics. This allows us to anticipate results in frame theory by using results from classical Mechanics.

How to construct unit norm tight frames effectively and computationally? We are devoted to new ideas of constructing tight frames for $\mathbb{R}^n$ that at the same time form spherical two-distance sets.

A finite collection of vectors $S = \{x_i, i \in I\} \subset \mathbb{R}^n$ is called a *finite frame* for the Euclidean space $\mathbb{R}^n$ if there are constants $0 < A \leq B < \infty$ such that for all $x \in \mathbb{R}^n$

$$A||x||^2 \leq \sum_{i \in I} |\langle x, x_i \rangle|^2 \leq B||x||^2.$$

If $A = B$, then S is called an A-tight frame. If in addition $||x_i|| = 1$ for all $i \in I$, then S is a unit-norm tight frame or FUNTF. If at the same time S is a spherical two-distance set, we call it a *two-distance tight frame*. In particular, if the two inner products in S satisfy the condition $a = -b$, then it is an equiangular tight frame or ETF.

Frames have been used in signal processing and have a large number of applications in sampling theory, wavelet theory, data transmission, and filter banks [25, 55, 56].

Motivated by the research on ETFs, we study frames that are at the same time two-distance sets and FUNTFs. Assume that the values of the inner product between distinct vectors in S are either a or b. We prove that the distance distribution of the frame with respect to any vector is the same (i.e., the Gram matrix G contains the same number of as in every row). Using this fact, we establish a new relation between two-distance FUNTFs and strongly regular graphs (SRGs). In the particular case of ETFs our connection enables us to recover the earlier examples in [81] as well as obtain some new examples of ETFs. We also make a few remarks on the parameters of ETFs and strongly regular graphs. We also notice that, Bannai [10], Cameron [24] and Neumaier [69] discussed embedding SRGs into spherical spaces to construct two-distance sets and spherical t-designs. Our approach is different from theirs and we can archive more examples of two-distance tight frames.

1.5 Nonexistence of spherical tight designs of harmonic index 4

The notion of spherical t-designs is introduced in (1.4). Tight spherical designs usually offer good structures and interesting configurations on spheres, but they exist vary rarely [8], [9]. If we consider generalizations of spherical designs, we may also get some interesting subsets of spheres. Therefore, if we consider the weaker version of spherical t designs, namely (1.4) only true for $\mathrm{Harm}_t(\mathbb{R}^n)$, then we call them spherical designs of harmonic index t. The explicit definition is as follows:

Definition 1.2 *A spherical design of harmonic index t is a finite subset $X \subset S^{n-1}$ such that*

$$\sum_{x \in X} f(x) = 0 \quad \forall f(x) \in \mathit{Harm}_t(\mathbb{R}^n). \tag{1.7}$$

The LP bound for spherical designs of harmonic index t was derived in [11]. If the bounds are attained, then designs are called tight. In particular, [11] shows that a tight design of harmonic index 4 gives arise to an equiangular line sets in $\mathbb{R}^n$ with angle $\arccos \sqrt{\frac{3}{n+4}}$ and cardinality $\frac{(n+1)(n+2)}{6}$. We prove that such equiangular line sets do not exist by deriving new relative bounds (Theorem 5.1) for equiangular line sets. We prove the bounds on cardinality of tight spherical design of harmonic index 4 strictly less than $\frac{(n+1)(n+2)}{6}$ and consequently there are no tight spherical designs of harmonic index 4. The technique to derive new relative bounds is a modification of the semidefinite programming method. Therefore, Theorem 5.1 is tighter than the classical relative bound (3.3) in [58].

It arouses our attention that the notion of spherical designs of harmonic index 2 are equivalent to tight frames. The proof is straightforward. If X is a spherical design of harmonic index 2, then by addition formula

$$\sum_{x_i,x_j\in X} G_2^n(\langle x_i, x_j\rangle) = 0.$$

Since $G_2^n(t) = \frac{nt^2-1}{n-1}$, we will have

$$\sum_{x_i,x_j\in X} |\langle x_i, x_j\rangle|^2 = \frac{|X|^2}{n}.$$

By [18], we know that this condition implies that X is a tight frame. Spherical 2-designs are spherical designs of harmonic index 2 and harmonic index 1. Therefore, spherical 2-designs are tight frames which also satisfy

$$\sum_{x_i,x_j\in X} \langle x_i, x_j\rangle = 0.$$

1.6 Contributions of this dissertation

- In Chapter 2, we discuss our contribution to spherical-two distance sets. We use the semidefinite programming method to compute improved estimates of the maximum size of spherical two-distance sets. Exact answers are found for dimensions $n = 23$ and $40 \leq n \leq 93$ $(n \neq 46, 78)$ where previous results gave divergent bounds. These results are published in [13].

- Chapter 3 contains our contribution for determining the maximum size of equiangular line sets in $\mathbb{R}^n$. Improvements are obtained in dimensions $24 \leq n \leq 136$. In particular, we show that the maximum number of equiangular lines in $\mathbb{R}^n$ is 276 for all $24 \leq n \leq 41$ and is 344 for $n = 43$. This provides a partial resolution of the conjecture set forth by Lemmens and Seidel (1973). These results are published in [14].

- Chapter 4 is devoted to finite two-distance tight frames. We derive new structural properties of the Gram matrix of a two-distance set that also forms a tight frame for $\mathbb{R}^n$. Our main results is a new correspondence between two-distance tight frames and certain strongly regular graphs. This allows us to use spectral properties of strongly regular graphs to construct two-distance tight frames. Several new examples are obtained using this characterization. These results are in the paper [15].

- Chapter 5 is concerned with new upper bound of the cardinality of a set of equiangular lines with the angle $\arccos(1/(2k-1))$ in the Euclidean space of dimension $12k^2 - 12k - 1$ for each integer $k \geq 2$. As a corollary to our bound, we show the nonexistence of spherical tight designs of harmonic index 4 on S^{n-1} with $n \geq 3$. We also derive new relative bounds for equiangular line sets which are tighter than classical relative bounds in [58]. The results appear in [70].

Chapter 2

New bounds for spherical two-distance sets

A spherical two-distance set is a finite collection of unit vectors in $\mathbb{R}^n$ such that the distances between any two distinct vectors assume only two values. We use the semidefinite programming method to compute improved estimates of the maximum size of spherical two-distance sets. Exact answers are found for dimensions $n = 23$ and $40 \le n \le 93$ $(n \ne 46, 78)$ where previous results gave divergent bounds.

2.1 Introduction

This chapter is devoted to the application of the semidefinite programming method to estimates of the size of the largest possible two-distance set on the sphere $S^{n-1}(\mathbb{R})$. A spherical two-distance set is a finite collection $\mathcal{C}$ of unit vectors in $\mathbb{R}^n$ such that the set of distances between any two distinct vectors in $\mathcal{C}$ has cardinality two. Estimating the maximum size $g(n)$ of such a set is a classical problem in distance geometry that has been studied for several decades.

We begin with an overview of known results. A lower bound on $g(n)$ is obtained as follows. Let $e_1, \dots, e_{n+1}$ be the standard basis in $\mathbb{R}^{n+1}$. The points $e_i + e_j, i \ne j$ form a spherical two-distance set in the plane $x_1 + \dots + x_{n+1} = 2$ (after scaling), and therefore

$$g(n) \ge n(n+1)/2, \quad n \ge 2. \tag{2.1}$$

The first major result for upper bounds was obtained by Delsarte, Goethals, and Seidel [36]. They proved that, irrespective of the actual values of the distances, the following "harmonic" bound holds true:

$$g(n) \le n(n+3)/2. \tag{2.2}$$

They also showed that this bound is tight for dimensions $n = 2, 6, 22$ in which cases it is related to sets of equiangular lines in dimension $n + 1$. Moreover, the results of [36], Bannai et al. [9], and Nebe and Venkov [67] imply that $g(n)$ can attain the harmonic bound only if $n = (2m + 1)^2 - 3, m \ge 1$ with the exception of an infinite sequence of values of m that begins with $m = 3, 4, 6, 10, 12, 22, 38, 30, 34, 42, 46$. Therefore, unless n is of the above form, $g(n) \le n(n + 3)/2 - 1$. These results are proved using the link between 2-distance sets and tight spherical 4-designs established in [36].

Another advance in estimating the function $g(n)$ was made by Musin [66]. Let $\mathcal{C} = \{z_1, z_2, \dots\}$ and suppose that $z_i \cdot z_j \in \{a, b\}, i \ne j$, where $2 - 2a, 2 - 2b$ are the values of the squared distances between the points. Musin proved that

$$|\mathcal{C}| \le n(n+1)/2 \quad \text{if } a + b \ge 0. \tag{2.3}$$

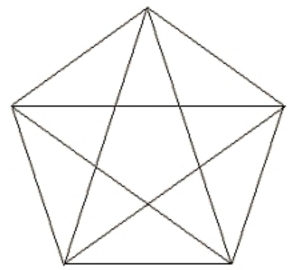

Figure 2.1: The maximum spherical two-distance set in $\mathbb{R}^2$: Pentagon.

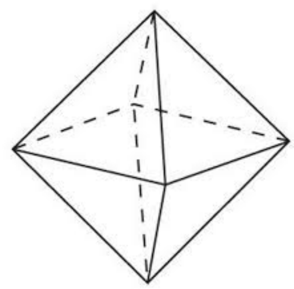

Figure 2.2: The maximum spherical two-distance set in $\mathbb{R}^3$: Octahedron.

He then used Delsarte's linear programming method to prove that $g(n) = n(n+1)/2$ if $7 \le n \le 39, n \ne 22, 23$.

Here we make another step for spherical two-distance sets, extending the range of dimensions in which the bound (2.3) is tight. The state of the art for $g(n)$ can be summarized as follows.

Theorem 2.1 *We have* $g(2) = 5, g(3) = 6, g(4) = 10, g(5) = 16, g(6) = 27, g(22) = 275,$

$$n(n+1)/2 \le g(n) \le n(n+3)/2 - 1, \quad n = 46, 78 \tag{2.4}$$

$$g(n) = n(n+1)/2, \quad 7 \le n \le 93, n \ne 22, 46, 78, \tag{2.5}$$

and $4465 \le g(94) \le 4492$. *If* $n \ge 95$, *then* $g(n) \le n(n+3)/2$ *or* $n(n+3)/2 - 1$ *as detailed in the remarks after Eq.* (2.2) *above.*

The part of this theorem that is established in the present paper relates to dimensions $n = 23$ and $40 \le n \le 94, n \ne 46, 78$. Our results are computational in nature and are obtained using the semidefinite programming method. The other parts of this theorem follow from the results in [36, 9, 66, 67]. The maximum spherical two-distance set in $\mathbb{R}^2$ is the Pentagon shown in Fig 2.1 and $\mathbb{R}^3$ is the Octahedron shown in Fig 2.2.

As far as actual constructions of spherical two-distance sets are concerned, rather little is known beyond the set of midpoints of the edges of a regular simplex mentioned above. Another way of constructing such sets is to start with a set of equiangular lines in $\mathbb{R}^n$ [58]. If the angle between each pair of lines is α, then taking one point from each pair of points on S^{n-1} defined by the line, we obtain a two-distance set with $a = \alpha, b = -\alpha$. The largest possible number of equiangular lines in $\mathbb{R}^n$ is $n(n+1)/2$ (this result is due to Gerzon, see [58]). This bound is attained for $n = 3, 7, 23$. For instance, for $n = 3$ the set of 6 lines is obtained from 6 diagonals of the icosahedron, which gives many ways of constructing inequivalent spherical two-distance sets of cardinality 6. The only three instances in which the known spherical two-distance sets are of cardinality greater than $n(n+1)/2$ occur in dimensions $n = 2, 6$ and 22.

2.2 Positive definite matrices and SDP bounds

A semidefinite program is an optimization problem of the form

$$\max\{\langle X, C\rangle \mid X \succeq 0,\ \langle X, A_i\rangle = b_i, i = 1, \dots, m\}, \tag{2.6}$$

where X is an $n \times n$ variable matrix, $A_1, \dots, A_m$ and C are given Hermitian matrices, $(b_1, \dots, b_m)$ is a given vector and $\langle X, Y\rangle = \operatorname{trace}(Y^* X)$ is the inner product of two matrices. Semidefinite programming is an extension of linear programming that has found a range of applications in combinatorial optimization, control theory, distance geometry, and coding theory. General introduction to semidefinite programming is given, for instance, in [17].

The main problem addressed by the SDP method in distance geometry is related to deriving bounds on the cardinality of point sets in a metric space $\mathcal{X}$ with a given set of properties such as a given minimum separation between distinct points in the set. The SDP method has its roots in harmonic analysis of the isometry group of the metric space in question. It is broadly applicable in both finite and compact infinite spaces. Examples of the former include the Hamming and Johnson spaces, their q-analogs, other metric spaces on the set of n-strings over a finite alphabet, as well as the finite projective space. The main example in the infinite case is given by real and complex spheres, although the SDP method is also applicable in other compact homogeneous spaces. Working out the details in each example is a nontrivial task that includes analysis of irreducible modules in the space of functions $f : \mathcal{X} \to \mathbb{C}$ under the action of the isometry group G of $\mathcal{X}$. The zonal matrices that arise in this analysis initially have large size that can be reduced relying on symmetries arising from the group action. This gives rise to an SDP optimization problem that is solved by computer for a given set of dimensions (the numerical part is also not straightforward and rather time-consuming). Foundations and analysis of particular cases have been the subject of a considerable number of research and overview publications in the last decade; see in particular recent surveys [4, 3] and references therein.

The origins of the SDP method and the discussed applications can be traced back to the work of Delsarte [35] which introduced the machinery of association schemes in the analysis of point configurations (codes) in finite spaces. Delsarte derived linear programming (LP) bounds on the cardinality of a set of points in the space under the condition on the minimum separation of distinct points in the set. Delsarte's results were linked to harmonic analysis and group representations in the works of Delsarte, Goethals and Seidel [36] (for the case S^{n-1}) and Kabatyansky and Levenshtein [53] (for general compact symmetric spaces).

From now on we focus on the case $\mathcal{X} = S^{n-1}$. Let $G_k^{(n)}(t), k = 0, 1, \dots$ denote the Gegenbauer polynomials of degree k. They are defined recursively as follows: $G_0^{(n)} \equiv 1, G_1^{(n)}(t) = t$, and

$$G_k^{(n)}(t) = \frac{(2k+n-4)tG_{k-1}^{(n)}(t) - (k-1)G_{k-2}^{(n)}(t)}{k+n-3}, \quad k \geq 2. \tag{2.7}$$

Delsarte et al. [36] showed that for any finite set of points $\mathcal{C} \subset S^{n-1}$

$$\sum_{(x,y)\in\mathcal{C}^2} G_k^{(n)}(x \cdot y) \geq 0, \quad k = 1, 2, \dots. \tag{2.8}$$

The proof of this inequality in [36] used the addition formula for spherical harmonics. An earlier, geometric proof of (2.8) had been given by Schoenberg [72], although his work was not known to researchers in the area discussed until at least the 1990s.

Positivity conditions (2.8) give rise to the LP bound on the cardinality of spherical two-distance sets.

Theorem 2.2 (Delsarte et al. [36]) *Let $\mathcal{C} \subset S^{n-1}$ be a finite set and suppose that $x \cdot y \in \{a, b\}$ for any $x, y \in \mathcal{C}$. Then*

$$|\mathcal{C}| \le \max\Big\{1 + \alpha_1 + \alpha_2 : \ 1 + \alpha_1 G_i^{(n)}(a) + \alpha_2 G_i^{(n)}(b) \ge 0, i = 0, 1, \dots, p; \alpha_j \ge 0, j = 1, 2\Big\}.$$

In this theorem α_1, α_2 are the optimization variables that refer to the number of ordered pairs of points in $\mathcal{C}$ with inner product a and b, respectively. For instance, $\alpha_1 = |\mathcal{C}|^{-1}\sharp\{(z_1, z_2) \in \mathcal{C}^2 : z_1 \cdot z_2 = a\}$, This theorem is a specialization of a more general LP bound on spherical codes of [36, 53].

Applications of semidefinite programming in coding theory and distance geometry gained momentum after the pioneering work of Schrijver [73] that derived SDP bounds on codes in the Hamming and Johnson spaces. Schijver's approach was based on the so-called Terwilliger algebra of the association scheme and formed a far-reaching generalization of the work of Delsarte [35]. Elements of the groundwork for SDP bounds in the Hamming space were laid by Dunkl [38], although this connection was also made somewhat later [79]. We refer to [62] for a detailed general survey of the approach via association schemes and further references.

SDP bounds for the real sphere were derived by Bachoc and Vallentin [5] in the context of the kissing number problem. The kissing number $k(n)$ is the maximum number of unit spheres that can touch a unit sphere without overlapping, i.e. the maximum number of points on the sphere such that the angular separation between any pair of them is at least $\pi/3$. Following [5], define a $(p-k+1) \times (p-k+1)$ matrix $Y_k^n(u, v, t), k \ge 0$ by setting

$$(Y_k^n(u, v, t))_{ij} = u^i v^j ((1-u^2)(1-v^2))^{k/2} G_k^{(n-1)}\Big(\frac{t - uv}{\sqrt{(1-u^2)(1-v^2)}}\Big)$$

where p is a positive integer, and a matrix $S_k^n(u, v, t)$ by setting

$$S_k^n(u, v, t) = \frac{1}{6}\sum_\sigma Y_k^n(\sigma(u, v, t)), \tag{2.9}$$

where the sum is over all permutations on 3 elements. Note that $(S_k^n(1, 1, 1))_{ij} = 0$ for all i, j and all $k \ge 1$. One of the main results of [5] is that for any finite set of points $\mathcal{C} \subset S^{n-1}$

$$\sum_{(x,y,z)\in\mathcal{C}^3} S_k^n(x \cdot y, x \cdot z, y \cdot z) \succeq 0 \tag{2.10}$$

The matrices S_k^n play the role of the constraints A_i in the general SDP problem (2.6). Positivity constraints (2.9) give rise to a general SDP bound on the cardinality of point sets obtained in [5], where it was used to improve upper bounds on $k(n)$ in small dimensions. In the next section we state a specialization of this bound for the case of 2-distance sets.

As a final remark, we note that constraints (2.8) arise from the unrestricted action of G on S^{n-1}. Constraints (5.3) are obtained by considering only actions that fix an arbitrary given point on the sphere. Further SDP bounds can be obtained by considering zonal matrices that arise from actions that fix any given number of points; however even for two points, actual evaluation of the bounds requires significant computational effort [64].

2.3 The bounds

The general SDP bound on spherical codes of [5] specializes to our case as follows.

Theorem 2.3 *Let $\mathcal{C}$ be a spherical two-distance set with inner products a and b. Let p be a positive integer. The cardinality $|\mathcal{C}|$ is bounded above by the solution of the following semidefinite programming problem:*

$$1 + {}^1\!/\!{}_3 \max(x_1 + x_2) \tag{2.11}$$

subject to

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{3}\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}(x_1 + x_2) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}(x_3 + x_4 + x_5 + x_6) \succeq 0 \tag{2.12}$$

$$3 + G_i^{(n)}(a)x_1 + G_i^{(n)}(b)x_2 \geq 0, \quad i = 1, 2, \ldots, p \tag{2.13}$$

$$\begin{aligned} S_i^n(1,1,1) + S_i^n(a,a,1)x_1 + S_i^n(b,b,1)x_2 + S_i^n(a,a,a)x_3 \\ + S_i^n(a,a,b)x_4 + S_i^n(a,b,b)x_5 + S_i^n(b,b,b)x_6 \succeq 0, \quad i = 0, 1, \ldots, p \end{aligned} \tag{2.14}$$

$$x_j \geq 0, j = 1, \ldots, 6,$$

where $S_i(\cdot,\cdot,\cdot)$ are $(p-i+1)\times(p-i+1)$ matrices defined in (5.3)*.*

In this theorem the variables x_1, x_2 refer to the number of ordered pairs of vectors in $\mathcal{C}$ with inner product a and b respectively; namely we have $x_i = 3\alpha_i, i = 1, 2$. We note that the SDP problem seeks to optimize the same linear form as the LP problem, but adds more constraints on the configuration. Because of this, Theorem 2.3 usually gives tighter bounds than Theorem 2.2. This fact is evident from the table below and is also known from the calculation of kissing numbers in [5].

2.3.1 Calculation of the bound

Several remarks are in order. First, implementation of SDP for two-distance sets differs from earlier computations in [5, 64] in that in our case there are no limits on the minimum separation of the points. Next, we restrict our calculations to the case $p \leq 5$ as no improvement is observed for larger values. Finally, by a result Larman et al. 1.1, we obtain a family of SDP bounds parametrized by a. Since $b_k(a) \geq -1, a + b_k(a) < 0$, we get that $a \in I_k := [0, \frac{1}{2k-1})$. Moreover, if $-1 \leq b < a \leq 0$, then $|\mathcal{C}|$ cannot be large by the Rankin bounds [71], and if $a + b \geq 0$ then $|\mathcal{C}|$ is bounded by (2.3). We conclude as follows.

Theorem 2.4 *Let* SDP(a) *be the solution of the SDP problem* (2.11)-(2.14)*, where $b = b_k(a)$. Let $\mathcal{C}$ be a spherical two-distance set with inner products a, b, then*

$$|\mathcal{C}| \leq \begin{cases} n(n+1)/2, & a + b \geq 0 \\ \mathrm{SDP}(a), & a \in I_k \\ n+1, & -1 \leq b < a < 0. \end{cases}$$

For instance, for $n = 23, k = 3$ we obtain that $I_k = [0, 0.2)$. Partitioning I_k into a number of small segments, we plot the value SDP(a) as a function of a evaluated at the nodes of the partition. The result is shown in Fig 2.3. A part of the segment around the maximum appears in the right part of Fig 2.3. This computation gives an indication of the answer, but in principle the value SDP(a) could oscillate between the nodes of the partition. Ruling this out requires perturbation analysis of the SDP problem which is not immediate.

2.3.1.1 Dual problem

The dual problem of (2.11)-(2.14) has the following form.

$$1+\min\Big\{\sum_{i=1}^{p}\alpha_i+\beta_{11}+\langle F_0,S_0^n(1,1,1)\rangle\Big\} \tag{2.15}$$

subject to

$$\begin{pmatrix}\beta_{11} & \beta_{22}\\ \beta_{12} & \beta_{22}\end{pmatrix}\succeq 0$$

$$2\beta_{12}+\beta_{22}+\sum_{i=1}^{p}(\alpha_i G_i^{(n)}(a)+3\langle F_i,S_i^n(a,a,1)\rangle)\leq -1 \tag{2.16}$$

$$2\beta_{12}+\beta_{22}+\sum_{i=1}^{p}(\alpha_i G_i^{(n)}(b)+3\langle F_i,S_i^n(b,b,1)\rangle)\leq -1 \tag{2.17}$$

$$\beta_{22}+\sum_{i=0}^{p}\langle F_i,S_i^n(y_1,y_2,y_3)\rangle\leq 0 \tag{2.18}$$

where $(y_1,y_2,y_3)\in\{(a,a,a),(a,a,b),(a,b,b),(b,b,b)\}$

$\alpha_i\geq 0,\ F_i\succeq 0,\ i=1,\dots,p.$

We need to estimate from above the maximum value of this problem over $a\in I_k=[a_1,a_2]$. Accounting for a continuous value set of the parameter in SDP problems is a challenging task. We approach it by employing the sum-of-squares method. Constraints (2.16)-(2.18) impose positivity conditions on some univariate polynomials of a for $a\in I_k$. The following sequence of steps transforms the constraints to semidefinite conditions. Observe that a polynomial $f(a)$ of degree at most m satisfies $f(a)\geq 0$ for $a\in I_k$ if and only if the polynomial of degree at most $2m$

$$f^+(a)=(1+a^2)^m f\Big(\frac{a_1+a_2a^2}{1+a^2}\Big)\geq 0$$

for all $a\in\mathbb{R}$. Next, a polynomial nonnegative on the entire real axis can be written as a sum of squares, $f(x)=\sum_i r_i^2(x)$, where the r_i are polynomials. Further, by a result of Nesterov [68], a polynomial $f(x)$ of degree $2m$ is a sum of squares if and only if there exists a positive semidefinite matrix Q such that $f=XQX^t$, where $X=(1,x,x^2,\dots,x^m)$. Thus, constraints (2.16)-(2.18) can be transformed to semidefinite conditions.

As a result, we obtain an SDP problem that can be solved by computer. We solved the resulting problem for $7\leq n\leq 96$ using the Matlab toolbox SOSTOOLS [83] in the YALMIP environment [82]. An advantage in using SOSTOOLS is that it accepts a as an SDP variable, thereby accounting for all the values of a in the segment. Thus, we obtain the value $\max$ SDP(a), $a\in I_k$. However, this may impose excessive constraints on the value of the SDP problem because all the conditions for different values of a are involved at the same time. To work around this accumulation, we use a sub-partitioning of the segment I_k into smaller segments. For each of them, SOSTOOLS outputs the largest value of the minimum of the SDP problem over all a in the segment. It turns out that, in many cases, the maximum of these solutions is smaller than $\max$ SDP(a), $a\in I_k$ computed directly by the package. The estimates of the answer computed from the primal problem

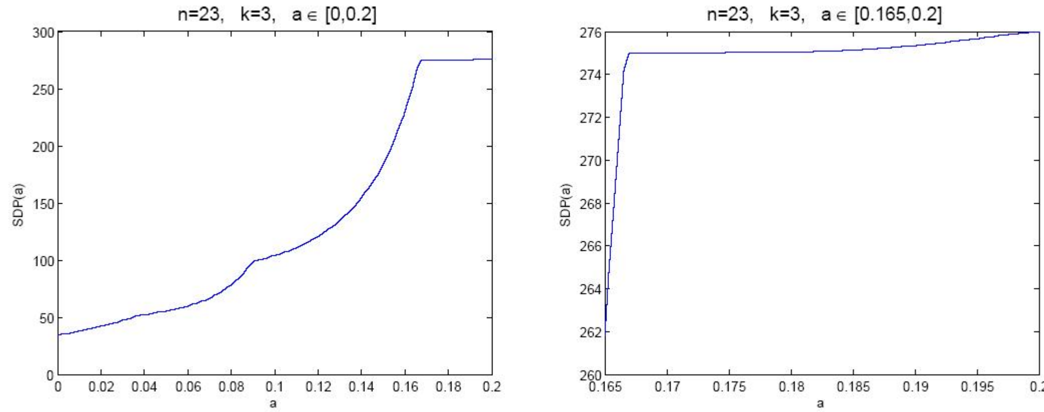

Figure 2.3: Evaluation of the SDP bound on $g(23)$

serve as a guidance of the needed step length of the partition. The solution of the sum-of-squares SDP optimization problem provides a rigorous proof for the estimates obtained by discretizing the primal problem (2.11)-(2.14). For instance, for $n = 23$ we partition I_3 into 20 subsegments, finding 276.5 as the maximum value of the dual SDP problem for $a \in I_3$, and similarly for other dimensions.

2.3.1.2 Results

The results of the calculation are summarized in the table below. The part of the table for $7 \leq n \leq 40$, except for the values of the SDP bound, is from [66]. The improvement provided by Theorem 2.3 over the LP bound is quite substantial even for relatively small dimensions. The LP bound is above $n(n+1)/2$ for $n \geq 40$ and is not included starting with $n = 41$. The cases $n = 46, 78$ and $n \geq 94$ are not resolved by SDP, although for $n = 94$ we still obtain an improvement over the harmonic bound (2.2). The value of k shown in the table accounts for the largest value of the SDP problem among the possible choices of k. This guarantees that the value SDP(a) is equal to or smaller than the number in the table for all the possible values of the inner products a, b in the point set.

Notice that for $n = 46, 78$ the SDP bound coincides with the bound (2.2). For $n = 23$ the results of [66] leave two possibilities, $g(n) = 276$ and 277. The SDP bound resolves this for the former, establishing the corresponding part of the claim in (4.3). As is seen from Fig 2.3, the largest value of SDP(a) is attained for $a = 0.2$ and is equal to 276. This case corresponds to 276 equiangular lines in $\mathbb{R}^{23}$ with angle $\arccos 0.2$, which can be constructed either using strongly regular graphs or the Leech lattice (see [58] for details).

Chapter 3

New bounds for equiangular lines

A set of lines in $\mathbb{R}^n$ is called equiangular if the angle between each pair of lines is the same. We address the question of determining the maximum size of equiangular line sets in $\mathbb{R}^n$, using semidefinite programming to improve the upper bounds on this quantity. Improvements are obtained in dimensions $24 \leq n \leq 136$. In particular, we show that the maximum number of equiangular lines in $\mathbb{R}^n$ is 276 for all $24 \leq n \leq 41$ and is 344 for $n = 43$. This provides a partial resolution of the conjecture set forth by Lemmens and Seidel (1973).

3.1 Introduction

A set of lines in a metric space is called equiangular if the angle between each pair of lines is the same. We are interested in upper bounds on the number of equiangular lines in $\mathbb{R}^n$. In other words, if we have a set of unit vectors $S = \{x_i\}_{i=1}^M$ and there is a constant $c > 0$ such that $|\langle x_i, x_j \rangle| = c$ for all $1 \leq i \neq j \leq M$, what is the maximum cardinality of S? Denote this quantity by $M(n)$. The problem of determining $M(n)$ looks elementary but a general answer has so far proved elusive: The maximum number of equiangular lines in $\mathbb{R}^n$ was known only for 16 values of the dimension n. The history of this problem started with Hanntjes [48] who found $M(n)$ for $n = 2$ and 3 in 1948. The pictures are shown in Fig 3.1 and Fig 3.2.

Van Lint and Seidel [60] found the largest number of equiangular lines for $4 \leq n \leq 7$. In 1973, Lemmens and Seidel [58] used linear-algebraic methods to determine $M(n)$ for most values of n in the region $8 \leq n \leq 23$. Gerzon (see [58]) gave the following upper on $M(n)$.

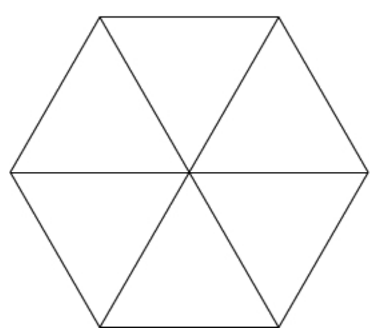

Figure 3.1: Maximum equiangular lines in $\mathbb{R}^2$: 3 lines through opposite vertices of a regular hexagon.

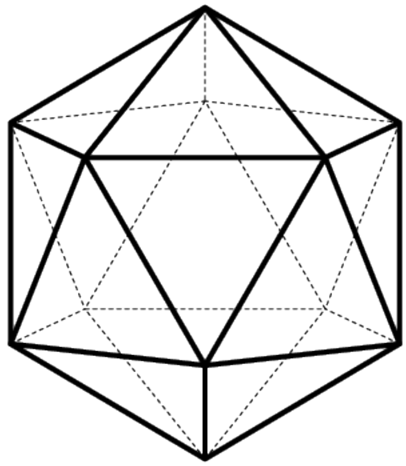

Figure 3.2: Maximum equiangular lines in $\mathbb{R}^3$: 6 lines through opposite vertices of an icosahedron.

Theorem 3.1 (Gerzon) *If there are M equiangular lines in $\mathbb{R}^n$, then*

$$M \leq \frac{n(n+1)}{2} \tag{3.1}$$

Gerzon's upper bound can be attained only for a very small number of values of n. Currently, such constructions are known only for $n = 2, 3, 7$, and 23. Neumann (see [58], Theorem 3.2) proved a fundamental result in this area:

Theorem 3.2 (Neumann) *If there are M equiangular lines in $\mathbb{R}^n$ with angle $\arccos\alpha$ and $M > 2n$, then $1/\alpha$ is an odd integer.*

Note that if M attains the Gerzon bound, then $(n+2)\alpha^2 = 1$ [58, Thm.3.5]. Therefore, if the cardinality of an equiangular line set attains the Gerzon bound, then n has to be 2 or 3 or an odd square minus two and the angle between pairs of lines is $\arccos 1/(\sqrt{n+2})$.

A set of unit vectors $S = \{x_1, x_2, \dots\} \subset \mathbb{R}^n$ is called *two-distance* if $\langle x_i, x_j\rangle \in \{a, b\}$ for some a, b and all $i \neq j$.

If the spherical two-distance set gives rise to equiangular lines, then $a = -b$, so Theorem 1.1 implies that $a = 1/(2k-1)$, which is the statement of the Neumann theorem. The assumption of Theorem 1.1 is more restrictive than of Theorem 3.2, but in return we obtain an upper bound on k. For instance, if $n = 40$, then k can be only 2 or 3, so the angle has to be $\arccos\alpha$, where $\alpha = 1/3$ or $1/5$. The assumption of Theorem 1.1 is satisfied since there exist equiangular line sets with $M \geq 2n+4$ for all $n \geq 15$.

The known bounds on $M(n)$ for small dimensions are summarized in Table 3.1 [58], [78], [45]; in particular, $M(n)$ was known exactly only if $2 \leq n \leq 13; n = 15, 21, 22, 23$. In the unsettled cases the best known upper bound in $M(n)$ is usually the Gerzon bound. Lemmens and Seidel [58, Thm. 4.5] further showed that

$$M_{1/3}(n) \leq 2(n-1), \quad n \geq 16, \tag{3.2}$$

where $M_\alpha(n)$ be the maximum size of an equiangular line set when the value of the angle is $\arccos\alpha$. They also conjectured that $M_{1/5}(n) = 276$ for $23 \leq n \leq 185$, observing that if this

n	$M(n)$	$1/\alpha$		n	$M(n)$	$1/\alpha$
2	3	2		17	48-50	5
3	6	$\sqrt{5}$		18	48-61	5
4	6	3; $\sqrt{5}$		19	72-76	5
5	10	3		20	90-96	5
6	16	3		21	126	5
$7 \leq n \leq 13$	28	3		22	176	5
14	28-29	$3; 5$		23	276	5
15	36	5		$24 \leq n \leq 42$	≥ 276	5
16	40-41	5		43	≥ 344	7

Table 3.1: Known bounds on $M(n)$ in small dimensions

n	$M(n)$	SDP bound		n	$M(n)$	SDP bound
3	6	6		18	48-61	61
4	6	6		19	72-76	76
5	10	10		20	90-96	96
6	16	16		21	126	126
$7 \leq n \leq 13$	28	28		22	176	176
14	28-29	30		23	276	276
15	36	36		$24 \leq n \leq 41$	276	276
16	40-41	42		42	≥ 276	288
17	48-50	51		43	344	344

Table 3.2: Bounds on $M(n)$ including new results

conjecture is true, then $M(n) = 276$ for $24 \leq n \leq 41$ and $M(43) = 344$. Note that generally we have [58]:

$$M_\alpha(n) \leq \frac{n(1-\alpha^2)}{1-n\alpha^2} \tag{3.3}$$

valid for all α such that the denominator is positive. This inequality is sometimes called the *relative bound* as opposed to the "absolute bound" of (3.1).

In this paper we use the semidefinite programming (SDP) method to derive some new bounds on $M(n)$. Our main results are summarized in Table 3.2. In particular, exact values of $M(n)$ are obtained for $24 \leq n \leq 41$ and for $n = 43$ where previous results gave divergent bounds: we show that $M(n) = 276$ for $24 \leq n \leq 41$ and $M(43) = 344$. These results are established by performing computations with SDP. We also show that $M_{1/5}(n) = 276$ for $23 \leq n \leq 60$. These results resolve a part of the Lemmens-Seidel conjecture and enable us to obtain the results in Table 3.2. For $44 \leq n \leq 136$, we also obtain new upper bounds on $M(n)$, improving upon the Gerzon bound, although no new exact values are found in this range. Below in the paper we give a more complete table of the computation results.

An interesting question relates to the asymptotic behavior of $M(n)$ for $n \to \infty$. For a long time the best known constructions were able to attain the growth order of $M(n) = \Omega(n)$, until D. de Caen [23] constructed a family of $\frac{2}{9}(n+1)^2$ equiangular lines in $\mathbb{R}^n$ for $n = 3 \cdot 2^{2t-1}, t \in \mathbb{N}$. Thus, currently the best asymptotic results are summarized as follows:

$$\frac{2}{9} \leq \limsup_{n\to\infty} \frac{M(n)}{n} \leq \frac{1}{2}, \tag{3.4}$$

where the upper bound is from (3.1). The question of the correct order of growth represents a difficult unresolved problem. Contributing to the study of the asymptotic bounds, we show that for $n = 3(2k-1)^2 - 4$ and $\alpha = \frac{1}{2k-1}$, for all integer $k \geq 2$,

$$M_\alpha(n) \leq \frac{(n+1)(n+2)}{6}. \tag{3.5}$$

3.2 SDP bounds for equiangular lines

Many problems in operations research, combinatorial optimization, control theory, and discrete geometry can be modelled or approximated as semidefinite programming. SDP optimization problems are usually stated in the following form:

$$\min c^T x$$

$$\text{subject to} \quad F_0 + \sum_{i=1}^{m} F_i x_i \succeq 0, \quad x \in \mathbb{R}^m,$$

where $c \in \mathbb{R}^m$ is a given vector of coefficients, $F_i, i = 0, 1, \dots$ are $n \times n$ symmetric matrices, and "$\succeq$" means that the matrix is positive semidefinite. SDP problems fall in the class of convex optimization problems since the domain of feasible solutions is a convex subset of $\mathbb{R}^m$. For the case of diagonal matrices F_i, SDP turns into a linear programming (LP) problem. Properties of SDP problems and algorithms for their solution are discussed, for instance, in [80]. Most SDP solvers such as CSDP, Sedumi, SDPT3 use interior point methods originating with Karmarkar's celebrated algorithm (We used CVX toolbox in Matlab.)

Let $\mathcal{C} \subset S^{n-1}$ be a set of unit vectors in $\mathbb{R}^n$ such that $\langle x, x' \rangle \leq a$ for all $x, x' \in \mathcal{C}, x \neq x'$ (a *spherical code*). As shown by Bachoc and Vallentin [5], the problem of estimating the maximum size of $\mathcal{C}$ can be stated as an SDP problem. In particular, for $a = 1/2$, this is the famous "kissing number problem", i.e., the question about the maximum number of nonoverlapping unit spheres that can touch a given unit sphere. A particular case of the main result in [5] was used in [13] to find new bounds on the maximum cardinality of spherical two-distance sets.

Let $G_k^{(n)}(t), k = 0, 1, \dots$ denote the Gegenbauer polynomials of degree k defined in (2.7) and a matrix $S_k^n(u, v, t)$ defined in (2.9). Using the approach of [13], we obtain the following SDP bound on $M(n)$.

Theorem 3.3 *Let $\mathcal{C}$ be a equiangular lines with inner product values either a or $-a$. Let p be the positive integer. The cardinality $|\mathcal{C}|$ is bounded above by the solution of the following semi-definite programming problem :*

$$1 + \frac{1}{3} \max(x_1 + x_2) \tag{3.6}$$

subject to

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{3} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} (x_1 + x_2) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} (x_3 + x_4 + x_5 + x_6) \succeq 0 \tag{3.7}$$

$$\begin{aligned} S_k^n(1,1,1) + S_k^n(a,a,1)x_1 + S_k^n(-a,-a,1)x_2 + S_k^n(a,a,a)x_3 \\ + S_k^n(a,a,-a)x_4 + S_k^n(a,-a,-a)x_5 + S_k^n(-a,-a,-a)x_6 \succeq 0 \end{aligned} \tag{3.8}$$

$$3 + G_k^{(n)}(a)x_1 + G_k^{(n)}(-a)x_2 \geq 0, \tag{3.9}$$

where $k = 0, 1, \cdots, p$ and $x_j \geq 0$, $j = 1, \cdots, 6$.

To compute bounds on $M(n)$, we found solutions of the SDP problem (3.6)-(3.9), restricting ourselves to the case our calculation to the case $p = 5$ since we need to cut the matrix size to be finite. In Table 3.3 we list the values of SDP bounds for all possible angles except the angle $\arccos \frac{1}{3}$ which is not included because of (3.2) (note that the SDP bounds for other angles are much greater than $2(n-1)$). The column labelled 'max' refers to the maximum of the SDP bounds among all possible angles. The last column in the table gives the value of the angle for which the maximum is attained.

Some comments on the tables are in order. Observe that $M_{1/5} = 276$ for $23 \le n \le 60$. Combined with the results of [58], this implies that $M(n) = 276$ for $23 \le n \le 41$ and $M(43) = 344$. The case $n = 42$ remains open since we only obtain that $276 \le M(42) \le 288$ for the angle $\arccos 1/7$.

Improvements of the Gerzon upper bound (3.1) are obtained for $n \le 136$. The last 3 entries in Table 3.3 produced no improvements, and are marked by an asterisk because of that. Similarly, the SDP problem yielded no improvements for higher dimensions.

An interesting, unexplained observation regarding this table is that the SDP bound for $M_\alpha(n)$ has long stable ranges for dimensions starting with the value $n = d^2 - 2$, where d is an odd integer and $\alpha = 1/d$. For instance, one such region begins with $d = 5$, another ones with $d = 7$. The same phenomenon can observed for $d = 9$ where the SDP value $M_\alpha(n) \le 3160$ is obtained for all values of n satisfying $79 \le n \le 227$ and for $d = 11$ where the value 7140 appears for all $n, 119 \le n \le 347$.

Note that the SDP bound gives the same value as the Gerzon bound for $n = 47, 79$ and 119, and that these three dimensions are of the form $n = (2k-1)^2 - 2$, where $k \ge 2$ is a positive integer. Bannai, Munemasa, and Venkov [9] showed that for $n = 47, 79$ the maximum possible size $M(n)$ cannot attain this value while the case $n = 119$ is still open. The result of [9] relies on the fact that an equiangular line set in $\mathbb{R}^n$ with cardinality $\frac{n(n+1)}{2}$ gives rise to a spherical two-distance set of size $(n-1)(n+2)/2$ in $\mathbb{R}^{n-1}$, and such sets are related to tight spherical 4-designs whose existence can be sometimes ruled out.

Based on the earlier results and our calculations, we make the following

CONJECTURE: *There exist* 1128 *equiangular lines in* $\mathbb{R}^{48}$ *with angle* $arccos(1/7)$ *and* 3160 *equiangular lines in* $\mathbb{R}^{80}$ *with angle* $arccos(1/9)$.

If this conjecture is true, then $M(n) = 1128$ for $48 \le n \le 75$ and $M(n) = 3160$ for $80 \le n \le 116$.

3.3 Tight spherical designs of harmonic index 4 and equiangular lines

The definitions of spherical designs and spherical designs of harmonic index t have been defined in (1.3) and (1.7).

The reason to define spherical design of harmonic index t is that we try to find weaker requirements of original spherical t design. Namely, spherical t designs require that (1.7) holds for $\mathrm{Harm}_i(\mathbb{R}^n)$ where $i = 1, 2, \cdots, t$, but spherical designs of harmonic index t only require $i = t$. An LP bound for spherical designs of harmonic index t was derived in [11]. Similarly, if this bound is attained, then the design is called tight.

Our interest in tight spherical designs of a fixed harmonic index is motivated by a result in [11] which shows that a tight design of index 4 gives rise to an equiangular line set in $\mathbb{R}^n$ with angle $\arccos a = \sqrt{3/(n+4)}$. Since $a = \frac{1}{2k-1}$ for some integer $k \ge 2$, we find that $n = 3(2k-1)^2 - 4$. These considerations motivate the following result.

n	1/5	1/7	1/9	1/11	1/13	1/15	max	Gerzon	angle
22	176	39	29	26	25	24	176	253	1/5
23	276	42	31	28	26	25	276	276	1/5
24	276	46	33	29	27	26	276	300	1/5
25	276	50	35	31	29	28	276	325	1/5
26	276	54	37	32	30	29	276	351	1/5
27	276	58	40	34	31	30	276	378	1/5
28	276	64	42	36	33	31	276	406	1/5
29	276	69	44	37	34	33	276	435	1/5
30	276	75	47	39	36	34	276	465	1/5
31	276	82	49	41	37	35	276	496	1/5
32	276	90	52	43	39	37	276	528	1/5
33	276	99	55	45	40	38	276	561	1/5
34	276	108	57	46	42	39	276	595	1/5
35	276	120	60	48	43	41	276	630	1/5
36	276	132	64	50	45	42	276	666	1/5
37	276	148	67	52	47	44	276	703	1/5
38	276	165	70	54	48	45	276	741	1/5
39	276	187	74	57	50	46	276	780	1/5
40	276	213	78	59	52	48	276	820	1/5
41	276	246	82	61	53	49	276	861	1/5
42	276	288	86	63	55	51	288	903	1/7
43	276	344	90	66	57	52	344	946	1/7
44	276	422	95	68	59	54	422	990	1/7
45	276	540	100	71	60	56	540	1035	1/7
46	276	736	105	73	62	57	736	1081	1/7
47	276	1128	110	76	64	59	1128	1128	1/7
48	276	1128	116	78	66	60	1128	1176	1/7
49	276	1128	122	81	68	62	1128	1225	1/7
50	276	1128	129	84	70	64	1128	1275	1/7
51	276	1128	136	87	72	65	1128	1326	1/7
52	276	1128	143	90	74	67	1128	1378	1/7
53	276	1128	151	93	76	69	1128	1431	1/7
54	276	1128	160	96	78	70	1128	1485	1/7
55	276	1128	169	100	81	72	1128	1540	1/7
56	276	1128	179	103	83	74	1128	1596	1/7
57	276	1128	190	106	85	76	1128	1653	1/7
58	276	1128	201	110	87	77	1128	1711	1/7
59	276	1128	214	114	90	79	1128	1770	1/7
60	276	1128	228	118	92	81	1128	1830	1/7
61	279	1128	244	122	94	83	1128	1891	1/7
62	290	1128	261	126	97	85	1128	1953	1/7
63	301	1128	280	130	99	87	1128	2016	1/7
64	313	1128	301	134	102	89	1128	2080	1/7
65	326	1128	325	139	105	91	1128	2145	1/7
66	339	1128	352	144	107	92	1128	2211	1/7
67	353	1128	382	148	110	94	1128	2278	1/7
68	367	1128	418	153	113	97	1128	2346	1/7

n	1/5	1/7	1/9	1/11	1/13	1/15	max	Gerzon	angle
69	382	1128	460	159	115	99	1128	2415	1/7
70	398	1128	509	164	118	101	1128	2485	1/7
71	416	1128	568	170	121	103	1128	2556	1/7
72	434	1128	640	176	124	105	1128	2628	1/7
73	453	1128	730	182	127	107	1128	2701	1/7
74	473	1128	845	188	130	109	1128	2775	1/7
75	494	1128	1000	195	134	112	1128	2850	1/7
76	517	1128	1216	202	137	114	1216	2926	1/9
77	542	1128	1540	210	140	116	1540	3003	1/9
78	568	1128	2080	217	144	118	2080	3081	1/9
79	596	1128	3160	225	147	121	3160	3160	1/9
80	626	1128	3160	234	151	123	3160	3240	1/9
81	658	1128	3160	243	154	126	3160	3321	1/9
82	693	1128	3160	252	158	128	3160	3403	1/9
83	731	1128	3160	262	162	130	3160	3486	1/9
84	772	1128	3160	272	166	133	3160	3570	1/9
85	816	1128	3160	283	170	136	3160	3655	1/9
86	866	1128	3160	294	174	138	3160	3741	1/9
87	920	1128	3160	307	178	141	3160	3828	1/9
88	979	1128	3160	320	182	143	3160	3916	1/9
89	1046	1128	3160	333	186	146	3160	4005	1/9
90	1120	1128	3160	348	191	149	3160	4095	1/9
91	1203	1128	3160	364	196	152	3160	4186	1/9
92	1298	1128	3160	380	200	154	3160	4278	1/9
93	1406	1128	3160	398	205	157	3160	4371	1/9
94	1515	1128	3160	417	210	160	3160	4465	1/9
95	1556	1128	3160	438	215	163	3160	4560	1/9
96	1599	1128	3160	460	220	166	3160	4656	1/9
97	1644	1128	3160	485	226	169	3160	4753	1/9
98	1691	1128	3160	511	231	172	3160	4851	1/9
99	1739	1128	3160	540	237	176	3160	4950	1/9
100	1790	1128	3160	571	243	179	3160	5050	1/9
101	1842	1128	3160	606	249	182	3160	5151	1/9
102	1897	1128	3160	644	255	185	3160	5253	1/9
103	1954	1128	3160	686	262	189	3160	5356	1/9
104	2014	1128	3160	734	268	192	3160	5460	1/9
105	2077	1128	3160	787	275	196	3160	5565	1/9
106	2142	1128	3160	848	282	199	3160	5671	1/9
107	2211	1128	3160	917	289	203	3160	5778	1/9
108	2282	1128	3160	997	297	206	3160	5886	1/9
109	2358	1128	3160	1090	305	210	3160	5995	1/9
110	2437	1128	3160	1200	313	214	3160	6105	1/9
111	2521	1128	3160	1332	321	218	3160	6216	1/9
112	2609	1128	3160	1493	330	222	3160	6328	1/9
113	2702	1128	3160	1695	339	226	3160	6441	1/9
114	2800	1128	3160	1954	348	230	3160	6555	1/9
115	2904	1128	3160	2300	357	234	3160	6670	1/9

n	1/5	1/7	1/9	1/11	1/13	1/15	max	Gerzon	angle
116	3015	1128	3160	2784	367	238	3160	6786	1/9
117	3132	1128	3160	3510	378	242	3510	6903	1/11
118	3257	1128	3160	4720	388	247	4720	7021	1/11
119	3390	1128	3160	7140	399	251	7140	7140	1/11
120	3532	1128	3160	7140	411	256	7140	7260	1/11
121	3684	1128	3160	7140	423	260	7140	7381	1/11
122	3848	1128	3160	7140	436	265	7140	7503	1/11
123	4024	1128	3160	7140	449	270	7140	7626	1/11
124	4214	1128	3160	7140	462	275	7140	7750	1/11
125	4419	1128	3160	7140	477	280	7140	7875	1/11
126	4643	1128	3160	7140	492	285	7140	8001	1/11
127	4887	1128	3160	7140	508	290	7140	8128	1/11
128	5153	1128	3160	7140	524	295	7140	8256	1/11
129	5447	1128	3160	7140	541	301	7140	8385	1/11
130	5770	1128	3160	7140	560	306	7140	8515	1/11
131	6130	1128	3160	7140	579	312	7140	8646	1/11
132	6531	1130	3160	7140	599	317	7140	8778	1/11
133	6982	1158	3160	7140	620	323	7140	8911	1/11
134	7493	1187	3160	7140	643	329	7493	9045	1/5
135	8075	1218	3160	7140	667	336	8075	9180	1/5
136	8747	1249	3160	7140	692	342	8747	9316	1/5
*137	9528	1282	3160	7140	719	348	9528	9453	1/5
*138	10450	1315	3160	7140	747	355	10450	9591	1/5
*139	11553	1350	3160	7140	778	362	11553	9730	1/5

Table 3.3: Values of the SDP bound on $M(n), 22 \leq n \leq 139$

Theorem 3.4 *Let $n = 3(2k-1)^2 - 4, k \geq 2$. The cardinality N of any equiangular line set in $\mathbb{R}^n$ with inner product $a = 1/(2k-1)$ satisfies the inequality*

$$|S| \leq \frac{(n+1)(n+2)}{6}. \tag{3.10}$$

Proof To prove this result we use the LP bound of [36] that has the following form: *Let $T \subset [-1,1]$. Let $S = \{x_1, x_2, \ldots, x_N\}$ be a set of unit vectors in $\mathbb{R}^n$ such $\langle x_i, x_j \rangle \in T \cup \{1\}$. Let $f(t) = \sum_k f_k G_k^n(t)$ be a polynomial such that $f_0 > 0, f_k \geq 0, k \geq 1$ and that $f(t) \leq 0$ for all $t \in T$. Then*

$$|S| \leq \left\lfloor \frac{f(1)}{f_0} \right\rfloor. \tag{3.11}$$

Consider the polynomial

$$f(t) = (t^2 - a^2)\Big(t^2 + \frac{a^2 n + 4a^2 - 6}{n+4}\Big).$$

Let $X \subset \mathbb{R}^n$ be an equiangular line set with inner product a. Then $T = \{\pm a\}$, and $f(t) = 0$ for $t \in T$. Computing the Gegenbauer expansion of $f(t)$, we obtain

$$\begin{aligned}
f_0 &= -\frac{a^4 n^2 + 6a^2 n(a^2-1) + 8a^4 - 6a^2(n+2) + 3}{n^2 + 6n + 8} \\
f_1 &= f_2 = f_3 = 0 \\
f_4 &= \frac{n^2 - 1}{(n+2)(n+4)}
\end{aligned}$$

We need to check that $f_0 > 0$. Substituting the values of n and a, we obtain

$$f_0 = \frac{8k(k-1)}{(2k-1)^4(12k^2 - 12k + 1)} \geq 0 \quad \text{for } k \geq 2.$$

Thus, $f(t)$ satisfies the conditions of the LP bound, and we obtain

$$|S| \leq \frac{f(1)}{f_0} = \frac{(a^2-1)(n+2)(n + a^2 n + 4a^2 - 2)}{a^4 n^2 + 6a^4 n + 8a^4 - 6a^2 n - 12a^2 + 3}.$$

In particular, putting $a = \frac{1}{2k-1}$ and $n = 3(2k-1)^2 - 4 = 12k^2 - 12k - 1$, we obtain

$$\frac{f(1)}{f_0} = \frac{(n+1)(n+2)}{6}.$$

This theorem gives infinitely many values of n for which the upper bound $M_a(n)$ is strictly less than the Gerzon bound, yielding the asymptotic constant 1/6 for the growth rate of the quantity $M_\alpha(n)$ (cf. (3.4)-(3.5)).

Remark 3.1 *Observe that the relative bound* (3.3) *is an instance of the LP bound* (3.11)*; see [36]. Thus, the SDP bound* (3.6)-(3.9) *is as strong or stronger than the bound* (3.3).

Remark 3.2 *Using SDP, we further show that for some dimensions the LP bound* (3.10) *cannot be attained. Indeed, for $k = 3, 4, 5$ we obtain the values of the dimension $n = 71, 143, 239$, respectively, and the SDP bound implies that*

$$M_{1/5}(71) \leq 416, \quad M_{1/7}(143) \leq 1506, \quad M_{1/9}(239) \leq 3902,$$

which is much smaller than the values $876, 3480, 9640$ *obtained from* (3.10). *Extending these calculations, we have shown that for* $k \leq 54$ *and* $n = 3(2k-1)^2 - 4 \leq 34343$ *the SDP bound improves upon the LP bound* (3.10).

In conclusion, we note that the value of the maximum in the LP problem for the maximum cardinality of equiangular line sets with a given angle can be explicitly characterized. The LP problem has the following form:

$$M_a(n) \leq \max\{1 + x_1 + x_2, x_1 \geq 0, x_2 \geq 0\} \tag{3.12}$$

subject to

$$1 + G_k^n(a)x_1 + G_k^n(-a)x_2 \geq 0 \quad \text{for } k = 1, 2, \ldots. \tag{3.13}$$

Theorem 3.5 *Let* $a \in (0,1)$,

$$g_n = \min_{k \geq 0} \frac{1}{|G_k^n(a)|} \tag{3.14}$$

where k *is even and such that* $G_k^n(a) < 0$*. Then*

$$M_a(n) \leq g_n + 1,$$

where the value $g_n + 1$ *is the solution of the LP problem* (3.12),(3.13).

Proof Let k be even, then $G_k^n(t)$ is an even function, so inequalities (3.13) take the form

$$1 + G_k^n(a)(x_1 + x_2) \geq 0, \quad k = 2m, m \in \mathbb{N}. \tag{3.15}$$

These inequalities define a set of half-planes whose boundaries are parallel to the objective function. The inequalities for odd k are bounded by lines that are perpendicular to the boundaries of the even-indexed constraints, and therefore can be disregarded. We conclude that the maximum is attained on the line $1 + G_k^n(a)(x_1 + x_2) = 0$ for some even k. The inequalities with k such that $G_k^n(a) \geq 0$ are trivially satisfied, therefore, we consider only those values of k when $G_k^n(a) < 0$. Eq. (3.15) implies that, for all even k,

$$x_1 + x_2 \leq -\frac{1}{G_k^n(a)} = \frac{1}{|G_k^n(a)|}.$$

This completes the proof.

To give an example of using this theorem, take $n = 71$ and $a = \frac{1}{5}$. To find a bound on $M_a(n)$, we estimate the quantity g_n in (3.14) by computing

$$\min_{0 \leq k \leq 100} \frac{1}{|G_k^{(71)}(1/5)|}$$

for all even k such that $G_k^{(71)}(1/5) < 0$. The smallest value is obtained for $k = 4$, and $G_4^{(71)}(1/5) = -1/875$. Thus, we obtain $M_{1/5}(71) \leq 876$. Of course, it could be possible that for greater k we obtain a smaller value of the bound, but this is not supported by our experiments (although we do not have a proof that $k = 4$ is the optimal choice).

Experiments also suggest that $k = 4$ may be the universal optimal choice for infinitely many values of n and a. Indeed, we have

$$G_4^n(x) = \frac{(n+2)(n+4)x^4 - 6(n+2)x^2 + 3}{n^2 - 1}.$$

Taking $n = 3(2t-1)^2 - 4$ and $a = 1/(2t-1)$, where $t \geq 2$, we obtain the expression

$$\frac{1}{G_4^n(a)} + 1 = 2t(t-1)(12t^2 - 12t + 1) = \frac{(n+1)(n+2)}{6}$$

which coincides with the LP bound (3.10).

Chapter 4

Two-distance tight frames

A finite collection of unit vectors $S \subset \mathbb{R}^n$ is called a spherical two-distance set if there are two numbers a and b such that the inner products of distinct vectors from S are either a or b. When $a + b \neq 0$, we derive new structural properties of the Gram matrix of a two-distance set that also forms a tight frame for $\mathbb{R}^n$. One of the main results of this paper is a new correspondence between two-distance tight frames and certain strongly regular graphs. This allows us to use spectral properties of strongly regular graphs to construct two-distance tight frames. Several new examples are obtained using this characterization.

4.1 Introduction

This chapter is devoted to new ideas of constructing spherical two-distance sets that at the same time form tight frames for $\mathbb{R}^n$.

4.1.1 Two-distance sets

A finite collection of unit vectors $S \subset \mathbb{R}^n$ is called a spherical two-distance set if there are two numbers a and b such that the inner products of distinct vectors from S are either a or b. If in addition $a = -b$, then S defines a set of equiangular lines through the origin in $\mathbb{R}^n$. Equiangular lines form a classical subject in discrete geometry following foundational papers of Van Lint, Seidel, and Lemmens [60, 58]. The main results in this area are concerned with bounding the maximum size $g(n)$ of the spherical two-distance set in n dimensions. A well-known general upper bound was obtained in the work of Delsarte et al. [36] who also constructed some examples of two-distance sets. Recently Musin [66] found the exact values of $g(n)$ for $7 \leq n \leq 39$ except the case $n = 23$. Barg and Yu [13] used the semidefinite programming method to resolve the case for dimension 23 as well as to obtain exact answers for $n \leq 93$ except the dimensions $n = 46, 78$. As far as constructions are concerned, the only known general method is rather trivial. Namely, let $e_1, \ldots, e_{n+1}$ be the standard basis in $\mathbb{R}^{n+1}$. The set

$$S = \{e_i + e_j, 1 \leq i < j \leq n + 1\} \tag{4.1}$$

forms a spherical two-distance set in the plane $x_1 + \cdots + x_{n+1} = 2$ (after scaling), and therefore $g(n) \geq n(n + 1)/2, n \geq 2$. Isolated examples of two-distance sets were constructed in [36, 61]. The following theorem summarizes the state of the art for $g(n)$ including the results of all the papers cited above.

Theorem 4.1 ([36, 61, 66, 13]) *We have* $g(2) = 5, g(3) = 6, g(4) = 10, g(5) = 16, g(6) = 27, g(22) = 275,$

$$n(n+1)/2 \leq g(n) \leq n(n+3)/2 - 1, \quad n = 46, 78 \tag{4.2}$$

$$g(n) = n(n+1)/2, \quad 7 \leq n \leq 93, n \neq 22, 46, 78, \tag{4.3}$$

and $4465 \leq g(94) \leq 4492$. *If* $n \geq 95$, *then* $n(n+1)/2 \leq g(n) \leq n(n+3)/2$ *(The upper bound here can sometimes be improved to* $n(n+3)/2 - 1$; *see [13] for details).*

This theorem shows that for most small values of the dimension n, construction (4.1) gives an optimally sized two-distance set.

4.1.2 Finite unit-norm tight frames (FUNTFs)

A finite collection of vectors $S = \{x_i, i \in I\} \subset \mathbb{R}^n$ is called a *finite frame* for the Euclidean space $\mathbb{R}^n$ if there are constants $0 < A \leq B < \infty$ such that for all $x \in \mathbb{R}^n$

$$A||x||^2 \leq \sum_{i \in I} |\langle x, x_i \rangle|^2 \leq B||x||^2.$$

If $A = B$, then S is called an A-tight frame. If in addition $||x_i|| = 1$ for all $i \in I$, then S is a unit-norm tight frame or FUNTF. If at the same time S is a spherical two-distance set, we call it a *two-distance tight frame*. In particular, if the two inner products in S satisfy the condition $a = -b$, then it is an equiangular tight frame or ETF.

The Gram matrix G of S is defined by $G_{ij} = \langle x_i, x_j \rangle, 1 \leq i, j \leq N$, where $N = |S|$. If S is a FUNTF for $\mathbb{R}^n$, then it is straightforward to show that G has one nonzero eigenvalue $\lambda = N/n$ of multiplicity n and eigenvalue 0 of multiplicity $N - n$, [50]

Frames have been used in signal processing and have a large number of applications in sampling theory, wavelet theory, data transmission, and filter banks [25, 55, 56]. The study of ETFs was initiated by Strohmer and Heath [77] and Holmes and Paulsen [52]. In particular, [52] shows that equiangular tight frames give error correcting codes that are robust against two erasures. Bodmann et al. [20] show that ETFs are useful for signal reconstruction when all the phase information is lost. Sustik et al. [78] derived necessary conditions on the existence of ETFs as well as bounds on their maximum cardinality.

Benedetto and Fickus [18] introduced a useful parameter of the frame, called the *frame potential*. For our purposes it suffices to define it as $FP(S) = \sum_{i,j=1}^{N} |\langle x_i, x_j \rangle|^2$. For a two-distance frame we obtain

$$\sum_{i,j=1}^{N} |\langle x_i, x_j \rangle|^2 = N + 2N_a a^2 + (N(N-1) - 2N_a)b^2, \tag{4.4}$$

where $N_a = |\{(i,j), i < j : \langle x_i \rangle x_j = a\}|$. Moreover, if $N > 2n + 1$, Theorem 1.1 implies that $b = (ka - 1)/(k - 1)$, where k is an integer between 2 and $(1/2)(1 + \sqrt{2n})$. This gives some information for a lower bound on $FP(S)$, but fortunately, a more general and concrete result is known from [18].

Theorem 4.2 *[18, Theorem.6.2] If* $N > n$ *then*

$$FP(S) \geq \frac{N^2}{n} \tag{4.5}$$

with equality if and only if S *is a tight frame.*

4.1.3 Previous research on frames and strongly regular graphs

The classic connection between equiangular line sets, 2-graphs, and strongly regular graphs (Seidel et al. [75, 36]; see also [41]) has been recently addressed in the context of frame theory, particularly in the study of ETFs [77, 52, 81]. The starting point of these studies can be summarized as follows. Let L be an equiangular line set with angles $a, -a$. Let us choose one vector on each of the lines of L (there are 2^N possible choices) and denote this set of vectors by $X = \{x_1, \dots, x_N\}$. Let $G = X^T X$ be the Gram matrix of X. Writing $G = I + aS$, we define the *Seidel matrix* S of the set X as a symmetric matrix with off-diagonal entries equal to ± 1. The Seidel matrix can be also thought of as an adjacency matrix of a graph on $|X|$ vertices, where -1 denotes adjacency and 1 denotes non-adjacency.

Next we note that it is possible to choose the vectors in L so that some fixed vector, say x_1, has the same angle a to all the other vectors in the set X. Indeed, if $\langle x_1, x_i \rangle = a$, then we include x_i in X, and otherwise if $\langle x_1, x_i \rangle = -a$, we include $-x_i$. This amounts to multiplying the matrix X by a diagonal matrix D with ± 1 on the diagonal so that the new matrix S' takes the form

$$S' = DSD = \begin{bmatrix} 0 & 1^T \\ 1 & \hat{S}' \end{bmatrix}. \tag{4.6}$$

In the language of graphs this operation is called Seidel switching, and the result of this switching is a graph in which vertex v_1 is isolated from the rest of the vertices. Generally, there are 2^N graphs that are switching equivalent, and the collection of these graphs is called a *switching class*. According to (4.6), the spectrum of S' is the same as the spectrum of S, so all the graphs in the switching class of X are co-spectral. The switching class of a graph is also known as a *two-graph*. By the above arguments, the spectrum of the two-graph is well-defined.

Now suppose that X is an ETF, then G has exactly two eigenvalues, namely N/n and 0, so the Seidel spectrum of the corresponding two-graph is $\{\frac{1}{a}(-1 + N/n), -1/a\}$. Two-graphs with two eigenvalues are called regular, and one of the basic results about them is that each of the matrices $\hat{S}'$ defined in (4.6) is the Seidel adjacency matrix of a strongly regular graph[1] [41, Thm. 11.6.1]. This enables one to use the known results about the existence of strongly regular graphs to construct new examples of ETFs. This line of thought was pursued in [52] and in particular in the recent work by Waldron [81], resulting in new examples of ETFs in $\mathbb{R}^n, n \le 50$. We note that some of the examples in [81] are two-distance frames, even though this paper did not emphasize the two-distance condition.

4.1.4 Contributions of this thesis

Motivated by the research on ETFs, in this thesis we study frames that are at the same time two-distance sets and FUNTFs. Assume that the values of the inner product between distinct vectors in S are either a or b. We prove that the distance distribution of the frame with respect to any vector is the same (i.e., the Gram matrix G contains the same number of as in every row). Using this fact, we establish a new relation between two-distance FUNTFs and strongly regular graphs, different from the connection discussed above, and find several examples of two-distance FUNTFs using this correspondence. In the particular case of ETFs our connection enables us to recover the earlier examples in [81] as well as obtain some new examples of ETFs. We also make a few remarks on the parameters of ETFs and strongly regular graphs.

[1] In the language of frame theory S (S') is called the (reduced) signature matrix of the frame.

4.2 Characterization of two-distance FUNTFs

First we show that the set of points (4.1) forms a FUNTF.

Proposition 4.1 *The set of all midpoints of the edges of a regular simplex in* $\mathbb{R}^{n+1}$ (4.1) *forms a two-distance FUNTF for* $\mathbb{R}^n$.

Proof Suppose that S is given by (4.1), then the inner products of distinct vectors in S are either 1 or 0. Let

$$N_{11} = |\{(i,j) : i < j,\ \langle e_1 + e_2, e_i + e_j \rangle = 1\}|$$

Observe that (i, j) is contained in this set if and only if $i = 1$ or $i = 2$, and we obtain $N_{11} = 2(n-1)$. By symmetry, the value N_{11} does not depend on the choice of the fixed vector $e_1 + e_2$, so the total number of (unordered) pairs of vectors in S with inner product 1 equals

$$N_1 = \frac{1}{2}\binom{n+1}{2} N_{11} = \frac{1}{2}(n-1)n(n+1).$$

The pairs of distinct vectors not counted in N_1 are orthogonal, and their count is

$$N_0 = \binom{n(n+1)/2}{2} - N_1 = \frac{1}{8}(n-2)(n-1)n(n+1).$$

Now let us project the vectors of S on the plane $x_1 + \cdots + x_{n+1} = 2$ and scale the result to place them on the unit sphere around the point $\frac{2}{\sqrt{n}}(1, 1, \ldots, 1)$. By Theorem 1.1 the obtained vectors have pairwise inner products that are either $a = (n-3)/(2(n-1))$ or $b = -2/(n-1)$. This information suffices to compute the frame potential, and we obtain

$$FP(S) = N + 2N_1 a^2 + 2N_0 b^2 = \frac{N^2}{n}$$

The frame potential meets the lower bound (4.5) with equality, which implies that S forms a FUNTF for $\mathbb{R}^n$.

In the remainder of this section we prove several characterization results for two-distance FUNTFs. Let $S \subset \mathbb{R}^n, |S| = N$ be a two-distance set with inner products a and b, $b < a$, and let $N_a = |\{(i,j) : i < j, x_i, x_j \in S, \langle x_i, x_j \rangle = a\}|$. We note that Theorems 1.1 and 4.2 give some necessary conditions for the existence of a two-distance FUNTF with the parameters n, N, a, N_a. However, we did not find them to be particularly useful, so we do not list them here.

The following theorem gives the value of N_a for a two-distance non-equiangular FUNTF.

Theorem 4.3 *Let G be the Gram matrix of a two-distance FUNTF $S \subset \mathbb{R}^n$ with inner products a and b such that $a + b \neq 0$. Then every column of G contains the same number of entries a and b, and the count of a's is given by*

$$N_a = \frac{\frac{N}{n} - 1 - (N-1)b^2}{a^2 - b^2}. \tag{4.7}$$

Proof G is similar to a diagonal matrix of order N with n nonzero entries $\lambda = N/n$ on the diagonal. Therefore, $G^2 - \lambda G = 0$, so $G^2 = \lambda G$ and the $(G^2)_{ii} = \lambda$ since $G_{ii} = 1$. We also have $(G^2)_{ii} = \sum_{j=1}^{N} G_{ij}^2$, so the norm of every row and of every column is the same and equals $\sqrt{\lambda}$.

Now let N_a be the number of entries a in any fixed column. Then

$$1 + a^2 N_a + b^2(N - 1 - N_a) = \frac{N}{n}.$$

This implies our claim.

If $a = -b$, then the statement of the theorem does not hold. Indeed, consider the set $S = \{x_1, \ldots, x_{28}\}$ of 28 vectors in $\mathbb{R}^7$ constructed according to (4.1). By Theorem 1.1 the inner products between distinct vectors in S are $\pm 1/3$, so they form a set of equiangular lines. For any given vector $x \in S$ we have $|\{y \in S : \langle x, y\rangle = 1/3\}| = 12$ and $|\{y \in S : \langle x, y\rangle = -1/3\}| = 15$. Now consider the set $S' = \{-x_1, x_2, \ldots, x_{28}\}$ which is also a FUNTF with inner products $\pm 1/3$, but the first column of G contains 12 entries equal to $-1/3$, which is different from all the other columns.

Our next result shows that the values of a and b for a two-distance FUNTF can be found directly, without recourse to Theorem 1.1.

Proposition 4.2 *Let S, is a non-equiangular two-distance tight frame in $\mathbb{R}^n$ of cardinality N with inner product values a or b. Then*

$$b = \frac{N + an - n}{n(a - aN - 1)} \quad \textit{or} \quad b = \frac{(N - n)(1 - a)}{N - n(a(N - 1) + 1)}.$$

Proof Theorem 4.3 implies that $\mathbf{1} = (11\ldots1)$ is an eigenvector of the Gram matrix G with eigenvalue 0 or N/n. Suppose it is the former, then $G \cdot \mathbf{1} = 0$, so the sum of entries in every row is 0. This implies that $1 + aN_a + (N - 1 - N_a)b = 0$, so from (4.7) we obtain the first of the two options for b in the statement.

Now suppose that $G \cdot \mathbf{1} = \frac{N}{n}\mathbf{1}$, so the sum of entries of G in any given row equals N/n. Repeating the calculation performed for the first case, we obtain the second of the two possibilities for b.

Finally, we note one more necessary condition for the existence of a two-distance tight frame implied by Theorem 1.1.

Proposition 4.3 *Let S be a two-distance non-equiangular FUNTF in $\mathbb{R}^n$ with N vectors, inner products a and b and N_a entries a in each row of the Gram matrix. Suppose that $N > 2n + 1$, then*

$$\frac{N(N-1)(ka-1)^2}{2(k-1)^2} - \frac{N_a}{(k-1)^2}((2k-1)a^2 - 2ka + 1) = \frac{N(N-n)}{2n}, \tag{4.8}$$

where $k \in \{2, \ldots, \lfloor (1 + \sqrt{2n})/2 \rfloor\}$.

Proof Indeed, let S be such a frame. Using the value of the frame potential found in (4.4) together with $b = (ka - 1)/(k - 1)$, we obtain

$$F_{N_a}(a) := \sum_{i<j}^{N} \langle x_i, x_j\rangle^2 = N_a a^2 + \Big(\frac{N(N-1)}{2} - N_a\Big)\Big(\frac{ka-1}{k-1}\Big)^2, \tag{4.9}$$

which is the same as the left-hand side of (4.8). At the same time, since $FP(S) = N^2/n = 2F_{N_a}(a) + N$. Consequently, $F_{N_a}(a) = \frac{N(N-n)}{2n}$ which conclude the proof. These necessary conditions on the parameters are really useful for small values of n. Indeed, if $n \le 12$, then k can take only the value 2, which enables us to rule out many sets of parameters.

4.3 Two-distance FUNTFs and strongly regular graphs

Connections between equiangular line sets and ETFs on the one side and strongly regular graphs on the other are well known and have been used in the literature to characterize the sets of parameters of ETFs [41, Ch. 11], [81]. In this section we extend this connection by relating two-distance (non equiangular) FUNTFs and strongly regular graphs in a new way.

We begin with a sufficient condition for the existence of two-distance FUNTFs. Let S be such a frame. The Gram matrix of any two-distance set with inner products a, b can be written as $G = I + a\Phi_1 + b\Phi_2$, where Φ_1 and Φ_2 are the corresponding indicator matrices. Letting J to be the matrix of all ones, we can write

$$G = (1-b)I + (a-b)\Phi_1 + bJ. \tag{4.10}$$

Note that $J^2 = NJ$ and $\Phi_1 J = N_a J$, where N_a is given by (4.7), and

$$G^2 = \frac{N}{n}G = \frac{N}{n}[(1-b)I + (a-b)\Phi_1 + bJ].$$

Therefore, squaring (4.10), we obtain a quadratic equation for Φ_1 :

$$(a-b)^2\Phi_1^2 + (a-b)\Big(2 - 2b - \frac{N}{n}\Big)\Phi_1 + \Big(2b(1-b) + b^2N + 2(a-b)bn_a - \frac{N}{n}b\Big)J \\ + (1-b)\Big(1 - b - \frac{N}{n}\Big)I = 0 \tag{4.11}$$

Note moreover that b is a function of a as described in Theorem 1.1. Therefore, we obtain the following claim.

Proposition 4.4 *Suppose that the values of N, n, and a are fixed. Let Φ_1 be a symmetric 0-1 matrix with the same number of 1s in every row that satisfies equation (4.11). Then there exists a two-distance FUNTF for $\mathbb{R}^n$ with N vectors whose Gram matrix is given by (4.10).*

Conversely, to each two-distance FUNTF for $\mathbb{R}^n$ with N vectors and inner products a, b is associated such a symmetric matrix Φ_1.

Proof The first part follows from the fact that given a matrix Φ_1 that satisfies these conditions, we can find a valid Gram matrix G and therefore, construct the configuration S.

The converse is straightforward.

This approach can be sometimes used to construct a 2-distance FUNTF. Consider the following example.

Example 4.1 *Let $n = 4, N = 10, a = 1/6$ and $b = -2/3$, then (4.11) takes the form $\Phi_1^2 + \Phi_1 - 2I - 4J = 0$. This gives the following relation for the entry (i, j) $(i \neq j)$ of Φ_1 :*

$$(\Phi_1^2)_{ij} + (\Phi_1)_{ij} - 4 = 0. \tag{4.12}$$

From (4.7) we find that $N_a = 6$. Without loss of generality assume that the first row of Φ_1 is 0111111000. Eq. (4.12) yields constraints on the rows 2 to 10 of Φ_1 : for instance, $(\Phi_1^2)_{12} = \sum_{l=1}^{10}(\Phi_1)_{1,l}(\Phi_1)_{2,l} = 3$, so we can assume that the second row of Φ_1 has the form 1011100110. Proceeding in this way, we can construct the rows of Φ_1 by trial and error. In this example, this approach succeeds, yielding the matrix

$$\Phi_1 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Now the Gram matrix G of a two-distance FUNTF S is found from (4.10)*, and the vectors of S can be found by constructing a 10×4 matrix F such that $FF^T = G$.*

This approach works well in small examples, but becomes computationally difficult as n and N increase because of the exponentially increasing search complexity. This motivates us to seek other methods of constructing the matrix Φ_1 that satisfies (4.11). Taking inspiration from the connection between ETFs and strongly regular graphs, e.g., [81], we use properties of the adjacency matrix of the graph as a tool for finding Φ_1.

A regular graph of degree k on v vertices is called strongly regular if every two adjacent vertices have λ common neighbors and every two non-adjacent vertices have μ common neighbors. Below we use the notation srg(v, k, λ, μ) to denote such strongly regular graph.

Theorem 4.4 ([41, p.219], [21, p.117]) *Let G be a graph on v vertices that is neither complete nor edgeless. Then G is strongly regular with the parameters (v, k, λ, μ) if and only if its adjacency matrix A satisfies the equation*

$$A^2 + (\mu - \lambda)A - \mu J + (\mu - k)I = 0. \tag{4.13}$$

For instance, the construction in Example 4.1 can be obtained from the adjacency matrix of strongly regular graph srg$(10, 6, 3, 4)$ because in this case Equation (4.13) coincides with (4.11).

Example 4.2 *Consider another example for $N = 25$. There exists a strongly regular graph srg$(25, 8, 3, 2)$ whose adjacency matrix therefore satisfies the equation*

$$A^2 - A - 2J - 6I = 0. \tag{4.14}$$

Aiming at constructing a two-distance FUNTF in $\mathbb{R}^8$ with $N = 25$ vectors and inner products $a = 3/8$ and $b = -1/4$, we note from (4.11) *that its matrix Φ_1 should satisfy Eq.* (4.14)*. Using the adjacency matrix A it is easy to construct the vectors of the frame S.*

Concluding, if a two-distance FUNTF and a strongly regular graph give rise to the same matrix equation, then one of these objects exists if and only if so does the other. We obtain the following result whose proof is immediate by comparing Equations (4.11) and (4.13).

Theorem 4.5 *A non-equiangular two-distance FUNTF (N, n, a, b) of cardinality N in $\mathbb{R}^n$ exists if and only if there exists a strongly regular graph with the parameters (v, k, λ, μ) where*

$$v = N, \quad k = c_2 + c_3, \quad \lambda = c_1 + c_2, \quad \mu = c_2, \tag{4.15}$$

where

$$c_1 = -\frac{2-2b-\frac{N}{n}}{a-b}, \quad c_2 = -\frac{2b(1-b)+b^2N+2(a-b)bN_a-\frac{N}{n}b}{(a-b)^2}$$
$$c_3 = -\frac{(1-b)(1-b-\frac{N}{n})}{(a-b)^2}$$

The four parameters of an srg(v, k, λ, μ) are not independent and must obey the following relation [41, p.119]:

$$k(k-1-\lambda) = \mu(v-k-1).$$

Together with the values of k, λ, μ in (4.15) this implies the following result.

Corollary 4.1 *A two-distance FUNTF with the parameters* (N, n, λ, μ) *exists only if*

$$(c_2+c_3)(c_3-c_1+1) = c_2(N-1-c_2-c_3).$$

CONSTRUCTING TWO-DISTANCE FUNTFS FOR SMALL DIMENSIONS. The approach outlined above suggests a way of constructing two-distance FUNTFs using the tables of known strongly regular graphs (see, e.g., [21, pp.143ff.] and the online tables [22]). Below in Table 4.1 we list examples obtained in this way for dimensions $4 \le n \le 10$, cardinality $N \le 50$, and inner products satisfying $b = 2a - 1$.

Rows of the table labelled by $*$ indicate that the FUNTFs in these rows have the largest possible cardinality as two-distance sets (cf. (4.3)). In the last two rows we list putative parameters of two-distance FUNTFs that would give rise to strongly regular graphs with the parameters $(50, 28, 18, 12)$. To the best of our knowledge, the existence of such graphs constitutes an open question. At the same time, (4.3) implies that spherical two-distance sets in dimensions $n = 7$ and 8 have cardinality at most $N = 36$. This implies that graphs srg$(50, 28, 18, 12)$ do not exist, which apparently was not known until this paper [22].

Table 4.1 includes several new examples of two-distance FUNTFs. For instance, the frame with the parameters $(N, n, a, b) = (25, 9, \frac{4}{9}, -\frac{1}{9})$ can be constructed from the srg$(25, 8, 3, 2)$, which is a product of two copies of K_5 (a complete graph on 5 vertices), etc. We also note that Bannai [10], Cameron [24], and Neumaier [69] showed that projection of the standard basis of $\mathbb{R}^n$ on the nontrivial eigenspaces of the adjacency matrix of an SRG yields a 2-distance set that also forms a spherical 2-design.

At the same time, this construction does not give two-distance tight frames that do not form spherical 2-designs. Using a different approach outlined in this section we obtain some new examples of two-distance tight frames.

4.4 Equiangular tight frames

In this section we examine the approach of this paper for the case of ETFs, i.e., the case when $b = -a$. In this case Theorem 1.1 implies that $a = 1/(2k-1)$ as long as the cardinality of the ETF satisfies $N > 2n+1$. At the same time, Theorem 5.1 does not apply in this case, so it may be possible to obtain ETFs from strongly regular graphs, but the existence of graphs does not form a necessary condition.

We say that S is an (N, n, a) ETF in $\mathbb{R}^n$ if it has cardinality N and inner products a and $-a$. We begin with a necessary condition for the existence of ETFs.

N	n	N_a	a	Quadratic equation	srg	comments
9	4	4	1/4	$A^2+A-2J-2I=0$	srg(9,4,1,2)	2-design
9	5	4	2/5	$A^2+A-2J-2I=0$	srg(9,4,1,2)	new
*10	4	6	1/6	$A^2+A-4J-2I=0$	srg(10,6,3,4)	Lisoněk [61]
10	5	3	1/3	$A^2+A-J-2I=0$	srg(10,3,0,1)	ETF
10	5	6	1/3	$A^2+A-4J-2I=0$	srg(10,6,3,4)	ETF
10	6	3	4/9	$A^2+A-J-2I=0$	srg(10,3,0,1)	new
15	5	8	1/4	$A^2-4J-4I=0$	srg(15,8,4,4)	Construction (4.1)
15	6	8	3/8	$A^2-4J-4I=0$	srg(15,8,4,4)	new
*16	5	10	1/5	$A^2-6J-4I=0$	srg(16,10,6,6)	Lisoněk
16	6	6	1/3	$A^2-2J-4I=0$	srg(16,6,2,2,)	ETF
16	6	10	1/3	$A^2-6J-4I=0$	srg(16,10,6,6)	ETF
16	7	6	3/7	$A^2-2J-4I=0$	srg(16,6,2,2,)	new
21	6	10	3/10	$A^2-A-4J-6I=0$	srg(21,10,5,4)	Construction (4.1)
21	7	10	2/5	$A^2-A-4J-6I=0$	srg(21,10,5,4)	new
25	8	8	3/8	$A^2-A-2J-6I=0$	srg(25,8,3,2)	2-design
25	9	8	4/9	$A^2-A-2J-6I=0$	srg(25,8,3,2)	new
*27	6	16	1/4	$A^2-2A-8J-8I=0$	srg(27,16,10,8)	Lisoněk [61]
27	7	16	5/14	$A^2-2A-8J-8I=0$	srg(27,16,10,8)	new
*28	7	12	1/3	$A^2-2A-4J-8I=0$	srg(28,12,6,4)	ETF
28	8	12	5/12	$A^2-2A-4J-8I=0$	srg(28,12,6,4)	new
*36	8	14	5/14	$A^2-3A-4J-10I=0$	srg(36,14,7,4)	Construction (4.1)
36	9	14	3/7	$A^2-3A-4J-10I=0$	srg(36,14,7,4)	new
36	10	10	2/5	$A^2-2A-2J-8I=0$	srg(36,10,4,2)	2-design
*45	9	16	3/8	$A^2-4A-4J-12I=0$	srg(45,16,8,4)	Construction (4.1)
45	10	16	7/16	$A^2-4A-4J-12I=0$	srg(45,16,8,4)	new
50	7	28	1/7	$A^2-6A-12J-16I=0$	srg(50,28,18,12)	does not exist
50	8	28	3/8	$A^2-6A-12J-16I=0$	srg(50,28,18,12)	does not exist

Table 4.1: Two-distance FUNTFs from graphs. The rows marked ‘new’ provide new examples of two-distance FUNTFs and marked ’2-design’ represent constructed in [69].

Proposition 4.5 *An $(N, n, a = \frac{1}{2k-1})$ ETF with $N > 2n+1$ vectors exists only if*

$$(N-n)(2k-1)^2 = (N-1)n, k = 2, 3, \dots, \lfloor (1+\sqrt{2n})/2 \rfloor.$$

Proof The quantity $F_N(a)$ in (4.9) (essentially, the frame potential) in this case equals $N(N-n)/2n$. At the same time, since S forms an equiangular line set, we have $F_N(a) = N(N-1)/2(2k-1)^2$.

Thus if an ETF in n dimensions exists, its cardinality can be found from this proposition. We list all the possible parameters of ETFs in $\mathbb{R}^n, n \le 60$ in Table 4.2. Two instances in the table, for $n = 17$ and $n = 54$ lead to matrix equations for Φ_1 with no solutions, so our approach is invalid.

In the remainder of this section we discuss one possible approach to the construction of ETFs. Let S be an ETF of cardinality N with inner products a and $-a$. Assume that the distance distribution of S with respect to any vector in it is the same, i.e., the number $|\{y \in S : \langle x, y\rangle = a\}|$ does not depend on $x \in S$. Then the Gram matrix $G(S)$ has the same number of entries equal to a in every row. Since the eigenvalues of G are N/n and 0, we have

$$G \cdot \mathbf{1} = \frac{N}{n} \quad \text{or} \quad G \cdot \mathbf{1} = 0,$$

or in other words

$$aN_a - a(N-1-N_a) + 1 = \frac{N}{n} \quad \text{or} \quad 0.$$

This gives just two possibilities for the value of N_a.

With this, it becomes possible to link ETFs and strongly regular graphs. For instance, taking $(N, n, a) = (36, 15, \frac{1}{5})$, we find that N_a is either 15 or 21. Now (4.11) implies that the matrix Φ_1 is a root of the quadratic equation

$$A^2 - 6J - 9I = 0 \quad \text{or} \quad A^2 - 12J - 9I = 0.$$

If it is the former, then recalling (4.13), we conclude that Φ_1 is the adjacency matrix of the graph srg(36,15,6,6). In the second case the parameters of the graph are $(36, 21, 12, 12)$. If either of these graphs exists, it gives rise to an ETF $(36, 15, \frac{1}{5})$.

In Table 4.2 we list the parameters of strongly regular graphs that are found using the above approach for all the possible parameters of ETFs with $n \leq 60$. The parameters of ETFs for $n \leq 47$ are cited from [27], which did not pursue the connection with strongly regular graphs.

Possible maximally sized ETFs: We note that for several of the sets of parameters that correspond to open cases in Table 4.2, their cardinality matches the best known upper bound on the size of equiangular line set in that dimension (the semidefinite programming, or SDP, bound of [14]). Specifically, this applies to $n = 19, 20, 42, 45, 46$. For instance, in the case of $n = 42$ the SDP bound gives $N = 288$ and $a = 1/7$ (it is not known whether a set of 288 equiangular lines in $\mathbb{R}^{42}$ exists). Using our approach, we observe that such a set could be constructed from srg(288,140,76,60) and srg(288,164,100,84). Unfortunately, neither of these two graphs is known to exist (or not). For two of the sets of graph parameters listed in the table, the graphs are known not to exist; however, this is not sufficient to claim the nonexistence of the corresponding ETFs.

k	n	N	a	comments
2	5	10	1/3	srg(10,3,0,1) (Y)
				srg(10,6,3,4) (Y)
2	6	16	1/3	srg(16,6,2,2) (Y)
				srg(16,10,6,6) (Y)
2	7	28	1/3	srg(28,12,6,4) (Y)
				srg(28,18,12,10) (Y)
3	15	36	1/5	srg(36,15,6,6) (Y)
				srg(36,21,12,12) (Y)
3	17	51	1/5	does not exist [78]
3	19	76	1/5	srg(76,45,28,24)(o)
				srg(76,35,18,14)(o)
3	20	96	1/5	srg(96,45,24,18) (o)
				srg(96,57,36,30) (N)
3	21	126	1/5	srg(126,60,33,24) (Y)
				srg(75,48,48,39) (Y)
3	22	176	1/5	srg(176,85,48,34) (Y)
				srg(176,105,68,54) (Y)
3	23	276	1/5	srg(276,135,78,54) (Y)
				srg(276,165,108,84) (N)
4	28	64	1/7	srg(64,28,12,12) (Y)
				srg(64,36,20,20) (Y)
4	33	99	1/7	does not exist [78]
4	35	120	1/7	srg(120,56,28,24) (Y)
				srg(120,68,40,36) (Y)
4	37	148	1/7	srg(148,70,36,30) (o)
				srg(148,84,50,44) (o)
4	41	246	1/7	srg(246,140,85,72) (o)
				srg(246,119,64,51) (o)
4	42	288	1/7	srg(288,140,76,60) (o)
				srg(288,164,100,84) (o)
4	43	344	1/7	srg(344,168,92,72) (Y)
				srg(344,196,120,100) (o)
4	45	540	1/7	srg(540,266,148,144) (o)
				srg(540,308,190,156) (N)
5	45	100	1/9	srg(100,45,20,20) (Y)
				srg(100,55,30,30) (Y)
4	46	736	1/7	srg(736,364,204,156) (o)
				srg(736,420,260,212) (o)
4	47	1128	1/7	does not exist [67]
5	51	136	1/9	srg(136,63,30,28) (Y) New
				srg(136,75,42,40)(Y)
5	54	160	1/9	does not exist [78]
5	57	190	1/9	srg(190,90,45,40) (o)
				srg(190,105,60,55) (o)

Table 4.2: Parameter sets of ETFs for $n \leq 60$. The label 'o' means that the existence of an SRG with these parameters is an open problem. 'Y' means that the corresponding ETF or a graph is known to exist and 'N' means that the srg does not exist. The cases of $n = 17, 54$ result in matrix equations (4.11) that have no solutions, so our method does not apply.

Chapter 5

Nonexistence of tight spherical designs of harmonic index 4

5.1 Introduction

The purpose of this chapter is to give a new upper bound of the cardinality of a set of equiangular lines with a certain angle (see Theorem 5.1). As a corollary to our upper bound, we show the nonexistence of spherical tight designs on harmonic index 4 on S^{n-1} with $n \geq 3$.

The notion of *a spherical design of harmonic index t on S^{n-1}* has been defined in (1.7). Our concern is tight harmonic index 4-designs. A harmonic index t-design X is *tight* if X attains the lower bound given by Theorem 2 in [11]. Especially, for the case $t = 4$, a harmonic index 4-design on S^{n-1} is tight if and only if its cardinality is $\frac{(n+1)(n+2)}{6}$.

For the case $n = 2$, we can construct tight harmonic index 4-designs as two points $\mathbf{x}$ and $\mathbf{y}$ on S^1 with the inner-product $\langle x, y\rangle = \sqrt{1/2}$. Theorem 5 in [11] studied nonexistence of tight harmonic index 4-design on higher-dimensional spheres and proved that if tight harmonic index 4-designs on S^{n-1} exists, then $n = 2$ or n must be of the form $n = 3(2k-1)^2 - 4 = 12k^2 - 12k - 1$ for some integer $k \geq 3$. It was also proved in [11] that a subset X of S^{n-1} with $|X| = \frac{(n+1)(n+2)}{6}$ is a tight harmonic index 4-design if and only if $I(X) \subset \{\pm\frac{1}{2k-1}\}$, where $I(X)$ is the set of inner-product values for all distinct pairs of the vectors in $X \subset \mathbb{R}^n$. Therefore, we derive the upper bounds on the cardinality of a set of equiangular lines with the angle $\arccos\frac{1}{2k-1}$ in $(12k^2 - 12k - 1)$-dimensional Euclidean space.

The main theorem of this section is as follows:

Theorem 5.1 *Let us fix an integer $k \geq 2$ and put $n_k := 3(2k-1)^2 - 4$ and $\alpha_k := \frac{1}{2k-1}$. Then for any finite subset X of S^{n_k-1} with $I(X) \subset \{\pm\alpha_k\}$, the inequality $|X| \leq 2(k-1)(4k^3 - k - 1)$ holds.*

Observe that

$$\frac{(n_k+1)(n_k+2)}{6} - 2(k-1)(4k^3-k-1) = 2(k-1)(2k-1)(4k^2-4k-1) \geq 0 \text{ when } k \geq 2.$$

Therefore, we have $\frac{(n_k+1)(n_k+2)}{6} > 2(k-1)(4k^3-k-1)$, when $k \geq 2$. In particular, we have the following corollary.

Corollary 5.1 *For each $n \geq 3$, there does not exist a tight harmonic index 4-design on S^{n-1}.*

Proof We use the notation $G_l^n(u)$ as Gegenbauer polynomials (2.7) and $S_l^n(u,v,t)$ as Zornal functions in [5]. It should be noted that the definition of $S_l^n(u,v,t)$ is different from that of Bachoc and Vallentin [6], and Barg and Yu [13] (see Remark 3.4 [5] for more on the differences).

The following computational result is used in the proof of Theorem 5.1:

Lemma 5.1 *For each $k \geq 2$,*

$$\begin{aligned}
(S_3^{n_k})_{1,1}(1,1,1) &= 0,\\
(S_3^{n_k})_{1,1}(\alpha_k,\alpha_k,1) &= (S_3^{n_k})_{1,1}(-\alpha_k,-\alpha_k,1) = 2(k-1)^2k^2(4k^2-4k-1)c_k.\\
(S_3^{n_k})_{1,1}(\alpha_k,\alpha_k,\alpha_k) &= (S_3^{n_k})_{1,1}(\alpha_k,-\alpha_k,-\alpha_k) = -3(k-1)^2c_k.\\
(S_3^{n_k})_{1,1}(\alpha_k,\alpha_k,-\alpha_k) &= (S_3^{n_k})_{1,1}(-\alpha_k,-\alpha_k,-\alpha_k) = -3k^2c_k.
\end{aligned}$$

where we put

$$c_k := \frac{216n_k(n_k+2)(n_k+6)}{(n_k-2)(n_k-1)(n_k+3)(n_k+4)^3}.$$

Note that c_k is a positive constant for each $k \geq 2$.

Proof To prove Lemma 5.1, we will need to give an explicit form of $(S_3^n)_{1,1}$

By the formula of S_l^n, we can compute that

$$\begin{aligned}
(S_3^n)_{1,1}(u,v,t) = &-\frac{n(n+2)(n+4)(n+6)}{3(n-2)(n-1)(n+1)(n+3)}((n-2)(u^4v^4+v^4t^4+t^4u^4)\\
&-3(nuvt+1)(u^2v^2+v^2t^2+t^2u^2)+3(u^4v^2+u^2v^4+v^4t^2+v^2t^4+t^4u^2+t^2u^4)\\
&+9(n+1)u^2v^2t^2-(n+7)uvt(u^2+v^2+t^2)+9uvt)
\end{aligned}$$

Especially, for any $\alpha \in (-1,1)$,

$$\begin{aligned}
(S_3^n)_{1,1}(1,1,1) &= 0\\
(S_3^n)_{1,1}(\alpha,\alpha,1) &= \frac{n(n+2)(n+4)(n+6)}{3(n-1)(n+1)(n+3)}\alpha^2(1-\alpha^2)^3\\
(S_3^n)_{1,1}(\alpha,\alpha,\alpha) &= -\frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)}(\alpha-1)^3\alpha^3((n-2)\alpha^2-6\alpha-3)\\
(S_3^n)_{1,1}(\alpha,\alpha,-\alpha) &= -\frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)}\alpha^3(\alpha+1)^3((n-2)\alpha^2+6\alpha-3).
\end{aligned}$$

In particular,

$$\begin{aligned}
(S_3^n)_{1,1}(\alpha,\alpha,1) &= (S_3^n)_{1,1}(-\alpha,-\alpha,1),\\
(S_3^n)_{1,1}(\alpha,\alpha,\alpha) &= (S_3^n)_{1,1}(\alpha,-\alpha,-\alpha),\\
(S_3^n)_{1,1}(\alpha,\alpha,-\alpha) &= (S_3^n)_{1,1}(-\alpha,-\alpha,-\alpha).
\end{aligned}$$

Lemma 5.1 follows.

Comment 5.1 *(Computational details for the entries of $S_l^n(u,v,t)$)*

We list the explicit terms in the entries of $S^n_l(u,v,t)$.

$$(S^n_3)_{1,1}(u,v,t) := \frac{1}{6}((Y^n_3)_{1,1}(u,v,t) + (Y^n_3)_{1,1}(u,t,v) + (Y^n_3)_{1,1}(t,v,u)) \qquad +$$

$$(Y^n_3)_{1,1} := \begin{cases} 0 \quad (\textit{ if } u = \pm 1 \textit{ or } v = \pm 1), \\ \lambda_{1,1} G^{n+6}_1(u) G^{n+6}_1(v) ((1-u^2)(1-v^2))^{3/2} G^{n-1}_3(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}) \quad (\textit{otherwise}) \end{cases}$$

$$\lambda_{1,1} = \frac{n(n+2)(n+4)}{(n-1)(n+1)(n+3)} h^{n+6}_1$$

$$h^{n+6}_1 := \dim \mathrm{Harm}_1(\mathbb{R}^{n+6}) = n+6$$

$$G^{n+6}_1(u) = u$$

$$G^{n-1}_3(t) = \frac{1}{n-2} t((n+1)t^2 - 3)$$

Hence

$$((1-u^2)(1-v^2))^{3/2} G^{n-1}_3(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}) = \frac{1}{n-2}(t-uv)((n+1)(t-uv)^2 - 3(1-u^2)(1-v^2))$$

$$\begin{aligned}(Y^n_3)_{1,1}(u,v,t) &= \frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)} uv(t-uv)((n+1)(t-uv)^2 - 3(1-u^2)(1-v^2)) \\ &= c'_n(uvt - u^2v^2)((n+1)t^2 - 2(n+1)uvt + (n-2)u^2v^2 + 3(u^2+v^2) - 3)) \\ &= -c'_n((n-2)u^4v^4 - 3(nuvt+1)u^2v^2 + 3u^2v^2(u^2+v^2) + 3(n+1)u^2v^2t^2 - 3uvt(u^2+v^2) \\ &\quad - (n+1)uvt^3 + 3uvt).\end{aligned}$$

where $c'_n := \frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)}$. *Therefore,*

$$\begin{aligned}(S^n_3)_{1,1}(u,v,t) &= -\frac{c'_n}{3}((n-2)(u^4v^4 + v^4t^4 + t^4u^4) - 3(nuvt+1)(u^2v^2 + v^2t^2 + t^2u^2) \\ &+ 3(u^4v^2 + u^2v^4 + v^4t^2 + v^2t^4 + t^4u^2 + t^2u^4) + 9(n+1)u^2v^2t^2 - (n+7)uvt(u^2+v^2+t^2) + 9uvt).\end{aligned}$$

We apply the SDP bound for spherical codes introduced by Bachoc and Vallentin [5] to spherical two distance sets. The explicit statement of it was given by Barg and Yu [13].

In order to state it, we define

$$\begin{aligned} W(x) &:= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}(x_1+x_2)/3 + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}(x_3+x_4+x_5+x_6), \\ S^n_l(x;\alpha,\beta) &:= S^n_l(1,1,1) + S^n_l(\alpha,\alpha,1)x_1 + S^n_l(\beta,\beta,1)x_2 + S^n_l(\alpha,\alpha,\alpha)x_3 \\ &\quad + S^n_l(\alpha,\alpha,\beta)x_4 + S^n_l(\alpha,\beta,\beta)x_5 + S^n_l(\beta,\beta,\beta)x_6 \end{aligned}$$

for each $x = (x_1,x_2,x_3,x_4,x_5,x_6) \in \mathbb{R}^6$ and $\alpha,\beta \in [-1,1)$. We remark that $W(x)$ is a symmetric matrix of size 2 and $S^n_l(x;\alpha,\beta)$ is a symmetric matrix of infinite size indexed by $\{(i,j) \mid i,j = 0,1,2,\ldots,\}$.

Fact 5.1 ([5] [13]) *Let us fix $\alpha,\beta \in [-1,1)$. Then any finite subset X of S^{n-1} with $I(X) \subset \{\alpha,\beta\}$ satisfies*

$$|X| \le \max\{1 + (x_1+x_2)/3 \mid x = (x_1,\ldots,x_6) \in \Omega^n_{\alpha,\beta}\}$$

where the subset $\Omega^n_{\alpha,\beta}$ *of* $\mathbb{R}^6$ *is defined by*

$$\Omega^n_{\alpha,\beta} := \{\, x = (x_1, \dots, x_6) \in \mathbb{R}^6 \} is defined by the following conditions.$$

1. $x_i \geq 0$ *for each* $i = 1, \dots, 6$.
2. $W(x) \succeq 0$ *i.e.* $W(x)$ *is positive semidefinite.*
3. $3 + G^n_l(\alpha)x_1 + G^n_l(\beta)x_2 \geq 0$ *for each* $l = 1, 2, \dots$.
4. *Any finite principal minor of* $S^n_l(x; \alpha, \beta)$ *is positive semidefinite for each* $l = 0, 1, 2, \dots$.

Thus, in order to prove Theorem 5.1, we only need to show the following proposition.

Proposition 5.1 *For each* $k \geq 2$*,*

$$\max\{1 + (x_1 + x_2)/3 \mid x \in \Omega^{n_k}_{\alpha_k, -\alpha_k}\} \leq 2(k-1)(4k^3 - k - 1). \tag{5.1}$$

Proof Let us take a positive semidefinite symmetric matrix

$$A(k) := \begin{pmatrix} (2k-1)^2(4k^3 - 2k^2 - 2k - 1)^2 & -(2k-1)(4k^3 - 2k^2 - 2k - 1) \\ -(2k-1)(4k^3 - 2k^2 - 2k - 1) & 1 \end{pmatrix}.$$

Since $W(x)$ is positive semidefinite for each $x \in \Omega^{n_k}_{\alpha_k, -\alpha_k}$, we have the trace of $(A(k) \cdot W(x))$ is non-negative, and then

$$(2k-1)^2(4k^3 - 2k^2 - 2k - 1)^2 - (16k^4 - 16k^3 - 4k^2 + 1)\frac{x_1 + x_2}{3}) + (x_3 + x_4 + x_5 + x_6) \geq 0. \tag{5.2}$$

Furthermore, $(S^{n_k}_3)_{1,1}(x; \alpha_k, -\alpha_k) \geq 0$ for each $x \in \Omega^{n_k}_{\alpha_k, -\alpha_k}$ since $(S^{n_k}_3)_{1,1}$ is a diagonal entry of $S^{n_k}_3$. Hence, by Lemma 5.1,

$$\frac{2}{3}k^2(k-1)^2(4k^2 - 4k - 1)(x_1 + x_2) - (k-1)^2(x_3 + x_5) - k^2(x_4 + x_6) \geq 0 \tag{5.3}$$

Therefore, by computing the sum of (5.2) and (5.3)$/(k-1)^2$, we have

$$\begin{aligned} &(2k-1)(4k^3 - 2k^2 - 2k - 1)((2k-1)(4k^3 - 2k^2 - 2k - 1) - \frac{x_1 + x_2}{3})) \\ &\geq (\frac{k^2}{(k-1)^2} - 1)(x_4 + x_6) \geq 0 \end{aligned}$$

Hence $2(k-1)(4k^3 - k - 1) \geq 1 + \frac{x_1 + x_2}{3}$ for any $x \in \Omega^{n_k}_{\alpha_k, -\alpha_k}$.

Remark 5.1 *Harmonic index* 4*-designs are defined by using the functional space* $\mathrm{Harm}_4(S^{n-1})$*. Therefore, it seems to be natural to consider* $\mathrm{Harm}_4(S^{n-1})$ *in the SDP method. In our proof, the functional space*

$$H^{n-1}_{3,4} \subset \bigoplus_{m=0}^{4} H^{n-1}_{m,4} = \mathrm{Harm}_4(S^{n-1})$$

(*see [5] for the definition of* $H^{n-1}_{m,l}$) *plays an important role to show the nonexistence of tight designs of harmonic index* 4 *since* $(S^n_3)_{1,1}$ *comes from* $H^{n-1}_{3,4}$*. We checked that if we consider* $H^{n-1}_{0,4} \oplus H^{n-1}_{1,4} \oplus H^{n-1}_{2,4} \oplus H^{n-1}_{4,4}$ *instead of* $H^{n-1}_{3,4}$*, our upper bound cannot be obtained for small* k*. However, we can not find any reasons of the importance of* $H^{n-1}_{3,4}$*.*

5.2 A new relative bound for equiangular lines

Theorem 5.1 *Let $n \geq 3$. Then the following holds:*

1.
$$M_\alpha(n) \leq 2 + (n-2)\frac{(1-\alpha)^3}{\alpha((n-2)\alpha^2 + 6\alpha - 3)}$$

for each $\alpha \in (0,1)$ with

$$(1-\alpha)^3(-(n-2)\alpha^2 + 6\alpha + 3) \geq (1+\alpha)^3((n-2)\alpha^2 + 6\alpha - 3) \geq 0.$$

2.
$$M_\alpha(n) \leq 2 + (n-2)\frac{(1+\alpha)^3}{\alpha(-(n-2)\alpha^2 + 6\alpha + 3)}$$

for each $\alpha \in (0,1)$ with

$$(1+\alpha)^3((n-2)\alpha^2 + 6\alpha - 3) \geq (1-\alpha)^3(-(n-2)\alpha^2 + 6\alpha + 3) \geq 0.$$

Example 5.1 *Let us consider the cases where $n_k := 3(2k-1)^2 - 4$ and $\alpha_k := 1/(2k-1)$ for an integer $k \geq 2$. Note that in such cases, Lemmens–Seidel's relative bound* (3.3) *does not work since $1 - n_k\alpha_k^2 = -2(4k^2 - 4k - 1)/(2k-1)^2 < 0$. One can compute that*

$$\begin{aligned}(1-\alpha_k)^3(-(n_k-2)\alpha_k^2 + 6\alpha_k + 3) &= \frac{96(k-1)^3 k}{(2k-1)^5},\\ (1+\alpha_k)^3((n_k-2)\alpha_k^2 + 6\alpha_k - 3) &= \frac{96(k-1)k^3}{(2k-1)^5},\end{aligned}$$

and hence

$$(1+\alpha_k)^3((n_k-2)\alpha_k^2 + 6\alpha_k - 3) \geq (1-\alpha_k)^3(-(n_k-2)\alpha_k^2 + 6\alpha_k + 3) \geq 0.$$

Therefore, by Theorem 5.1, we have

$$\begin{aligned}M_{\alpha_k}(n_k) &\leq 2 + (n-2)\frac{(1+\alpha)^3}{\alpha(-(n-2)\alpha^2 + 6\alpha + 3)}\\ &= 2(k-1)(4k^3 - k - 1).\end{aligned}$$

In order to prove Theorem 5.1, we only need to show the following proposition.

Proposition 5.2 *Let $n \geq 3$ and $0 < \alpha < 1$. Then the following holds:*

1.
$$\max\{1 + (x_1 + x_2)/3 \mid x \in \Omega^n_{\alpha,-\alpha}\} \leq 2 + 2 + (n-2)\frac{(1-\alpha)^3}{\alpha((n-2)\alpha^2 + 6\alpha - 3)} \tag{5.4}$$

if $(1-\alpha)^3(-(n-2)\alpha^2 + 6\alpha + 3) \geq (1+\alpha)^3((n-2)\alpha^2 + 6\alpha - 3) \geq 0$.

2.
$$\max\{1 + (x_1 + x_2)/3 \mid x \in \Omega^n_{\alpha,-\alpha}\} \leq 2 + (n-2)\frac{(1+\alpha)^3}{\alpha(-(n-2)\alpha^2 + 6\alpha + 3)} \tag{5.5}$$

if $(1+\alpha)^3((n-2)\alpha^2 + 6\alpha - 3) \geq (1-\alpha)^3(-(n-2)\alpha^2 + 6\alpha + 3) \geq 0$.

Proof We need an explicit formula of $(S_3^n)_{1,1}$. For each $-1 < \alpha < 1$,

$$
\begin{aligned}
(S_3^n)_{1,1}(1,1,1) &= 0 \\
(S_3^n)_{1,1}(\alpha,\alpha,1) &= \frac{n(n+2)(n+4)(n+6)}{3(n-1)(n+1)(n+3)}\alpha^2(1-\alpha^2)^3 \\
(S_3^n)_{1,1}(\alpha,\alpha,\alpha) &= -\frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)}(\alpha-1)^3\alpha^3((n-2)\alpha^2-6\alpha-3) \\
(S_3^n)_{1,1}(\alpha,\alpha,-\alpha) &= -\frac{n(n+2)(n+4)(n+6)}{(n-2)(n-1)(n+1)(n+3)}\alpha^3(\alpha+1)^3((n-2)\alpha^2+6\alpha-3).
\end{aligned}
$$

Fix α with $0 < \alpha < 1$. We take $x \in \Omega^n_{\alpha,-\alpha}$ For simplicity we put $X = (x_1 + x_2)/3$, $Y = x_3 + x_5$ and $Z = x_4 + x_6$. Since $W(x)$ is positive semidefinite, by taking its determinant, we have

$$
-X(X-1) + Y + Z \geq 0. \tag{5.6}
$$

Furthermore, we have $(S_3^n)_{1,1}(x;\alpha,-\alpha) \geq 0$ since $(S_3^n)_{1,1}$ is a diagonal entry of S_3^n. Hence,

$$
(n-2)\frac{(1-\alpha^2)^3}{\alpha}X-(1-\alpha)^3(-(n-2)\alpha^2+6\alpha+3)Y-(1+\alpha)^3((n-2)\alpha^2+6\alpha-3)Z \geq 0 \tag{5.7}
$$

Therefore, in the cases where

$$
(1-\alpha)^3(-(n-2)\alpha^2+6\alpha+3) \geq (1+\alpha)^3((n-2)\alpha^2+6\alpha-3) \geq 0,
$$

we obtain

$$
(n-2)\frac{(1-\alpha^2)^3}{\alpha}X - (1+\alpha)^3((n-2)\alpha^2+6\alpha-3)(Y+Z) \geq 0.
$$

By (5.6),

$$
(n-2)\frac{(1-\alpha^2)^3}{\alpha}X - (1+\alpha)^3((n-2)\alpha^2+6\alpha-3)X(X-1) \geq 0
$$

Thus we have

$$
2 + (n-2)\frac{(1-\alpha)^3}{\alpha((n-2)\alpha^2+6\alpha-3)} \geq X + 1 = 1 + (x_1+x_2)/3.
$$

By the similar arguments, in the cases where

$$
(1+\alpha)^3((n-2)\alpha^2+6\alpha-3) \geq (1-\alpha)^3(-(n-2)\alpha^2+6\alpha+3) \geq 0,
$$

we have

$$
2 + (n-2)\frac{(1+\alpha)^3}{\alpha(-(n-2)\alpha^2+6\alpha+3)} \geq X + 1 = 1 + (x_1+x_2)/3.
$$

5.3 Calculation details for Theorem 5.1

This section is devoted to offer the calculation details that how do we construct the matrix $A(x)$.

Lemma 5.2 *Let us put $x = (x_1, x_2, x_3, x_4, x_5, x_6)$ be a point in $\mathbb{R}^6$ satisfying the three conditions below:*

1. $x_i \geq 0$ *for each* $i = 1, \ldots, 6$.
2. $2(k-1)^2k^2(4k^2-4k-1)(x_1+x_2) - 3(k-1)^2(x_3+x_5) - 3k^2(x_4+x_6) \geq 0$.
3. $W(x) := \begin{pmatrix} 1 & (x_1+x_2)/3 \\ (x_1+x_2)/3 & (x_1+x_2)/3 + (x_3+x_4+x_5+x_6) \end{pmatrix} \succeq 0.$

Then the inequality below holds:

$$1 + (x_1+x_2)/3 \leq 2(k-1)(4k^3-k-1).$$

For simplicity we put $h_k := 2(k-1)^2k^2(4k^2-4k-1)$.
Goal : $(m-1)x_0^* - (x_1^* + x_2^*)/3$
Assume that $A(x) := \begin{pmatrix} a & b \\ b & c \end{pmatrix} \succeq 0$, then $a \geq 0$, $c \geq 0$, $b^2 \leq ac$. Then,

$$\begin{aligned} & h_k(x_1^*+x_2^*)/3 - (k-1)^2(x_3^*+x_5^*) - k^2(x_4^*+x_6^*) + ax_0^* + (2b+c)(x_1^*+x_2^*)/3 + c(x_3^*+x_4^*+x_5^*+x_6^*) \\ &= ax_0^* + (2b+c+h_k)(x_1^*+x_2^*)/3 + (c-(k-1)^2)(x_3^*+x_5^*) + (c-k^2)(x_4^*+x_6^*). \end{aligned}$$

We want to minimize $1 + a/(-2b-c-h_k)$ with $0 \leq a$, $0 \leq c \leq (k-1)^2$, $b^2 \leq ac$ and $-2b-c-h_k < 0$. We can put $a = b^2/c$. Then,

$$\begin{aligned} 1 + \frac{a}{-2b-c-h_k} &= 1 + \frac{b^2}{-2cb-c^2-ch_k} \\ &= \frac{5}{4} - \frac{b}{2c} + \frac{h_k}{4c} + \frac{(c^2+2ch_k+h_k^2)}{4c(-2b-c-h_k)} \\ &= \frac{5}{4} + \frac{h_k}{4c} - \frac{b}{2c} + \frac{(c+h_k)^2}{4c(-2b-c-h_k)} \\ &= \frac{5}{4} + \frac{h_k}{4c} + \frac{4c(-2b-c-h_k)}{16c^2} + \frac{c+h_k}{4c} + \frac{(c+h_k)^2}{4c(-2b-c-h_k)} \\ &= \frac{5}{4} + \frac{c+2h_k}{4c} + \frac{4c(-2b-c-h_k)}{16c^2} + \frac{(c+h_k)^2}{4c(-2b-c-h_k)} \\ &\geq \frac{5}{4} + \frac{c+2h_k}{4c} + 2\sqrt{\frac{4c(-2b-c-h_k)}{16c^2} \cdot \frac{(c+h_k)^2}{4c(-2b-c-h_k)}} \\ &\quad \text{(The equality holds if and only if } b = -c-h_k) \\ &= \frac{5}{4} + \frac{c+2h_k}{4c} + \frac{c+h_k}{2c} \\ &= \frac{5}{4} + \frac{3c+4h_k}{4c} \\ &= 2 + \frac{h_k}{c}. \end{aligned}$$

Therefore,

$$1 + \frac{a}{-2b - c - h_k}$$

is minimized as

$$2 + \frac{h_k}{(k-1^2)} = 2 + 2k^2(4k^2 - 4k - 1) = 2(k-1)(4k^3 - k - 1).$$

at

$$\begin{aligned} &a = b^2/c = (k-1)^2(2k-1)^2(4k^3 - 2k^2 - 2k - 1)^2 \\ &b = -c - h_k = -(k-1)^2(2k-1)(4k^3 - 2k^2 - 2k - 1) \\ &c = (k-1)^2. \end{aligned}$$

Chapter 6

Summary and future work

In Chapter 2, we extend the known table of exact answers of maximum size of spherical two-distance sets in $\mathbb{R}^n$ for $n = 23$ and $40 \leq n \leq 93$. The method is the so-called three-point SDP method. We expect that if we use the four-point SDP method, then we can achieve exact answers for higher dimensions. The four-point SDP method has been used to get better results in the Hamming space by D. C. Gijswijt, H. D. Mittelmann and A. Schrijver in [40]. We are also interested in the estimation of maximum size of spherical two-distance sets in $\mathbb{R}^n$ for $n = 46$ and 78, which are the only two missing cases for $n \leq 93$ but it is not clear how to approach it.

In Chapter 3, we contribute to find the maximum size of equiangular line sets in $\mathbb{R}^n$ for $24 \leq n \leq 41$ and $n = 43$. It is interesting that we can determine most of the values of n, where $n \leq 43$, but $M(14)$ and $M(16)$ remain open up to two possible values, i.e. $M(14) = 28$ or 29 and $M(16) = 40$ or 41. Again, we expect that four-point SDP method can help to determine them. We observe that for the known maximum size of equiangular line sets in $\mathbb{R}^n$ are all even numbers. We conjecture that this is true for all n and if our conjecture holds, then $M(14) = 28$ and $M(16) = 40$.

An interesting, unexplained observation regarding Table 3.3 is that the SDP bound for $M_\alpha(n)$ has long stable ranges for dimensions starting with the value $n = d^2 - 2$, where d is an odd integer and $\alpha = 1/d$. For instance, $M_{1/5} = 276$ for $23 \leq n \leq 60$ and $M_{1/7} = 1128$ for $47 \leq n \leq 131$. Our new relative bounds may help to prove this phenomenon in general, but we have not yet completed the proof.

In Chapter 4, we derive new structural properties of the Gram matrix of a two-distance tight frames in $\mathbb{R}^n$ and have a new correspondence between two-distance tight frames and certain strongly regular graphs (SRGs). However, our constructions rely on the known table of SRGs. For instance, we want to construct an ETF with parameters $(N, n, \alpha) = (76, 19, 1/5)$ since we know that the upper bound of equiangular line sets in $\mathbb{R}^{19}$ is 76. If this ETF can be constructed, then we can determine $M(19) = 76$. However, the corresponding srg(76,35,18,14) is also an open problem for the existence. We have ideas to approach the constructions of ETFs without using SRGs, but that requires large-volume computation. We will attempt to use the ideas in this chapter to work on the structures of complex two-distance tight frames and complex ETFs.

In Chapter 5, we use a variation of the SDP method to derive new relative bounds for equiangular line sets in $\mathbb{R}^n$. Our motivation is coming from particular values of angles and dimensions. In [58], Lemmens and Seidel proved that $M_{1/3}(n) = 2(n-1)$ for $n \geq 16$. However, $M_{1/5}(n)$ remains open for a long period of time. $M_{1/7}(n)$ and other angles are also open. We expect that our new relative bounds or other variations of SDP can be used to derive a general bound on $M_{1/5}(n)$.

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