Four-point semidefinite bound for equiangular lines

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Abstract

A set of lines in $\mathbb{R}^d$ passing through the origin is called equiangular if any two lines in the set form the same angle. We proved an alternative version of the three-point semidefinite constraints developed by Bachoc and Vallentin, and the multi-point semidefinite constraints developed by Musin for spherical codes. The alternative semidefinite constraints are simpler when the concerned object is a spherical $s$-distance set. Using the alternative four-point semidefinite constraints, we found the four-point semidefinite bound for equiangular lines. This result improves the upper bounds for infinitely many dimensions $d$ with prescribed angles. As a corollary of the bound, we proved the uniqueness of the maximum construction of equiangular lines in $\mathbb{R}^d$ for $7 \leq d \leq 14$ with inner product $\alpha = 1/3$, and for $23 \leq d \leq 64$ with $\alpha = 1/5$.

1 Introduction

A set of lines in $\mathbb{R}^d$ passing through the origin is called equiangular if any two lines in the set form the same angle. We denote the maximum cardinality of sets of equiangular lines in $\mathbb{R}^d$ by $N(d)$. Searching the values of $N(d)$ is one of the classical problems in discrete geometry. The history can be traced back to 1948 by the work of Haantjes [23], who settled the problem for $d = 3$ and $d = 4$. To the best of our knowledge, the results for the bounds for $N(d)$ are summarized in Table 1; see Appendix A.1 for the details. One can also refer to Sequence A002853 in The On-Line Encyclopedia of Integer Sequences [38] for the latest results.

| $d$ | 2  | 3–4 | 5  | 6  | 7–14 | 15 | 16 | 17 |
|-----|----|-----|----|----|------|----|----|----|
| $N(d)$ | 3  | 6  | 10 | 16 | 28   | 36 | 40 | 48 |
| $d$ | 18 | 19 | 20 | 21 | 22   | 23–41 | 42 | 43 |
| $N(d)$ | 57–60 | 72–74 | 90–94 | 126 | 176   | 276 | 276–288 | 344 |

Table 1: The maximum cardinality of equiangular lines for small dimensions $d$

For a set of equiangular lines in $\mathbb{R}^d$, let $X \subseteq \mathbb{S}^{d-1}$ be a set of unit vectors constructed by choosing a unit vector along every line. Then the set $X$ satisfies

$$c \cdot c' = ±\alpha \quad \text{for all} \quad c, c' \in X \quad \text{and} \quad c \neq c'$$

for some real number $\alpha \in [0, 1)$. The set $X$ is called a spherical projection of the original set of equiangular lines. A spherical projection is a spherical 2-distance set, i.e., a set of unit vectors with the inner product set

$$A(X) := \{c \cdot c' : c, c' \in X, c \neq c'\}$$

containing two different elements. A set $X \subseteq \mathbb{S}^{d-1}$ of unit vectors is a spherical $s$-distance set if $|A(X)| = s$.  

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Let $N_\alpha(d)$ be the maximum cardinality of sets of equiangular lines in $\mathbb{R}^d$ with prescribed inner products $\pm \alpha$. Neumann \cite{27} proved that, for a set of equiangular lines in $\mathbb{R}^d$ with cardinality greater than $2d$, the reciprocal of the inner product $\alpha$ must be an odd integer. Therefore, the values of $N_{1/a}(d)$ for odd integers $a$ are essential for determining $N(d)$. Below are some partial results on $N_{1/a}(d)$; see Appendix A.2 for the details.

Lemmens and Seidel \cite{27} completely determined $N_{1/3}(d)$ for all dimensions $d$ as in Table 2. Note that the maximum cardinalities remain the same from $d = 7$ to $d = 15$, and become a linear function in $d$ for $d \geq 15$. There is a similar phenomenon when $\alpha = 1/5$: Cao et al. \cite{11} proved that $N_{1/5}(d) = 276$ for $23 \leq d \leq 185$, and $N_{1/5}(d) = \lfloor \frac{3}{2}(d-1) \rfloor$ for $d \geq 185$.

| $d$  | 3   | 4   | 5   | 6   | 7-15 | 15- |
|------|-----|-----|-----|-----|------|-----|
| $N_{1/3}(d)$ | 4   | 6   | 10  | 16  | 28   | $2d-2$ |

Table 2: The maximum cardinality of equiangular lines for $\alpha = 1/3$

In general, the asymptotic behaviors of $N_\alpha(d)$ are also determined.

**Theorem 1.1** (Jiang et al. \cite{26}). Let $a \geq 3$ be an odd integer. Then $N_{1/a}(d) = \lfloor \frac{a+1}{a-1}(d-1) \rfloor$ for all sufficiently large dimensions $d$.

As for the constant upper bound counterpart, there is a theorem proved by applying the three-point semidefinite programming method to spherical projections of sets of equiangular lines.

**Theorem 1.2** (Yu \cite{43}). Let $a \geq 3$ be an odd integer. Suppose $d \leq D_3(a) = 3a^2 - 16$. Then

$$N_{1/a}(d) \leq \frac{1}{2}(a^2 - 1)(a^2 - 2).$$

The three-point semidefinite programming method is initially developed by Bachoc and Vallentin \cite{3} to bound the kissing numbers in $\mathbb{R}^d$. The method consists of some constraints on the three-point distance distribution, i.e., the number of triples in a spherical set $X$ with three specified values for pairwise inner products. Theorem 1.2 is called the three-point semidefinite bound for equiangular lines.

The aim of this paper is to generalize Theorem 1.2. We consider the multi-point distance distributions, which must satisfy some constraints developed by Musin \cite{32}. We proved an alternative version of the semidefinite constraints. The alternative semidefinite constraints are simpler when the concerned object $X$ is a spherical $s$-distance set. When $X$ is a spherical projection of a set of equiangular lines, the constraints can be simplified further by considering the mutual relations of different spherical projections. We call this simplification by switching reduction. Using the alternative four-point semidefinite constraints with switching reduction, we proved the following four-point semidefinite bound for equiangular lines.

**Theorem 1.3.** Let $a \geq 3$ be an odd integer. Suppose $d \leq D_4(a) = 3a^2 + (12/\sqrt{5})a - 948/25 + o(1)$. Then

$$N_{1/a}(d) \leq \frac{1}{2}(a^2 - 1)(a^2 - 2).$$

The four-point semidefinite bound is a generalization of the three-point semidefinite bound, in the sense that Theorem 1.3 gives upper bounds for $N_{1/a}(d)$ for infinitely many pairs $(a, d)$ more than Theorem 1.2. To be specific, the largest applicable dimensions $d$ are improved from $D_3(a) = 3a^2 + O(1)$ to $D_4(a) = 3a^2 + (12/\sqrt{5})a + O(1)$. The improvements for small $a$ are shown in Table 3.
The four-point semidefinite bound agrees with the work by de Laat et al. [13]. They gave the upper bounds for $N_{1/a}(d)$ for $a = 5, 7, 9, 11$ by the four-point semidefinite programming method. By this method, they showed that $N_{1/5}(65) \leq 276$, $N_{1/7}(145) \leq 1128$, $N_{1/9}(251) \leq 3160$ and $N_{11}(381) \leq 7140$ numerically. Theorem 1.3 serves as a rigorous proof of their results and is applicable for infinitely many $a$.

If a set of equiangular lines is a maximum construction attaining the equality in Theorem 1.3, we can derive more information about it.

**Theorem 1.4.** Let $a \geq 3$ be an odd integer and $d < D_4(a)$. Then a set of equiangular lines in $\mathbb{R}^d$ with cardinality $(a^2 - 1)(a^2 - 2)/2$ and inner product $1/a$ must lie in an $(a^2 - 2)$-dimensional subspace.

By Theorem 1.4 along with the uniqueness of the strongly regular graphs with some specific parameters, we proved the uniqueness of the maximum construction of equiangular lines in $\mathbb{R}^d$ for $7 \leq d \leq 14$ with $\alpha = 1/3$, and for $23 \leq d \leq 64$ with $\alpha = 1/5$.

The article is organized as follows: In Section 2, we review the three-point semidefinite constraints developed by Bachoc and Vallentin [3], and the multi-point semidefinite constraints developed by Musin [32]. We also prove an alternative version of these constraints in Section 2. In Section 3 we develop the switching reduction on the regime that $X$ is a spherical projection of a set of equiangular lines. In Section 4 we give the proof of the main results, namely, Theorem 1.3 and Theorem 1.4. Section 5 contains some further questions.

In the following text, $X$ is a spherical $s$-distance set in $\mathbb{S}^{d-1}$ when not specified, and the cardinality is $N = |X|$. The inner product set of $X$ is defined by

$$A(X) := \{c \cdot c' : c, c' \in X, c \neq c'\}.$$ 

So $|A(X)| = s$. We also write $A'(X) = A(X) \cup \{1\}$. When it is specified that $X$ is a spherical projection of a set of equiangular lines in $\mathbb{R}^d$, we fix $A(X) = \{\pm \alpha\}$ and $a = 1/\alpha$.

## 2 Semidefinite constraints

The semidefinite programming method is developed by Bachoc and Vallentin [3]. This method is a generalization of the linear programming method developed by Delsarte et al. [14].

The two methods are initially developed to bound the kissing numbers in $\mathbb{R}^d$, that is, the maximum cardinality of $X \subseteq \mathbb{S}^{d-1}$ such that $A(X) \subseteq [-1, 1/2]$. In 1979, Odlyzko and Sloane [35] and Levenshtein [28] independently proved that the kissing numbers in $\mathbb{R}^8$ and $\mathbb{R}^{24}$ are 240 and 196560 using the linear programming method. Musin [31] proved that the kissing number in $\mathbb{R}^4$ is 24 by a modification of the linear programming method. Meanwhile, Bachoc and Vallentin [3] gave the same result by the semidefinite programming method.

The linear programming method and the semidefinite programming method involve the following parts:

| $a$ | $3$ | $5$ | $7$ | $9$ | $11$ |
|-----|-----|-----|-----|-----|-----|
| $D_3(a)$ | 11 | 59 | 131 | 227 | 347 |
| $D_4(a)$ | 14.42 | 64.56 | 144.52 | 250.41 | 380.96 |

Table 3: $D_3(a)$ and $D_4(a)$ for small $a$
1. Consider the distance distribution of a spherical set $X$.
2. The distance distribution is related to the cardinality $N = |X|$.
3. Meanwhile, the distance distribution satisfies some specific inequalities or semidefinite constraints.
4. The upper bound for the cardinality $N$ is given by considering a linear program or a semidefinite program with $N$ being the objective function and the distance distribution being the variables.

This framework can also be applied to spherical $s$-distance sets, as well as spherical projections of sets of equiangular lines. See [7, 8, 15, 36, 43] for some upper bounds on spherical 2-distance sets and equiangular lines proved by using the semidefinite programming method.

Bachoc and Vallentin’s semidefinite programming method involves the three-point distance distribution satisfying the so-called three-point semidefinite constraints. Musin [32] generalized the method and developed the multi-point semidefinite constraints of $(m+2)$-point distance distributions for $m \geq 1$. As an application, de Laat et al. [13] gave some numerical upper bounds on the cardinality of sets of equiangular lines by $(m+2)$-point semidefinite programming method for $1 \leq m \leq 4$.

In this section, we review the linear inequalities and the semidefinite constraints and prove an alternative version of the semidefinite constraints. The alternative semidefinite constraints (Theorem 2.3 and Theorem 2.13) are simpler than the original ones (Theorem 2.2 and Theorem 2.12) when the concerned object $X$ is a spherical $s$-distance set.

### 2.1 Two-point linear inequality

**Part 1.** Consider the two-point distance distribution

$$x(t) := \#\{(c, c') \in X^2 : c \cdot c' = t\}.$$  

The value $x(t)$ counts the number of pairs in $X$ with inner product $t$. Clearly $x(1) = N$, and $x(t) > 0$ only when $t = 1$ or $t \in A(X)$.

**Part 2.** $\sum_{t \in A(X)} x(t) = N(N-1)$.

**Part 3.** The inequalities for the distance distribution $x(t)$ arise from the property of a series of polynomials called Gegenbauer polynomials. The Gegenbauer polynomials $\{P^d_k(t) : k = 0, 1, 2, \ldots\}$ are defined by

$$P^d_0(t) = 1,$$
$$P^d_1(t) = t,$$
$$P^d_k(t) = \frac{1}{k+d-3} \left((2k+d-4)P^d_{k-1}(t) - (k-1)P^d_{k-2}(t)\right), \quad k \geq 2.$$  

For $c, c' \in S^{d-1}$, $P^d_k(c \cdot c')$ can be realized as a specific inner product (Delsarte et al. [14]). Therefore

$$\sum_{c, c' \in X} P^d_k(c \cdot c') \geq 0 \text{ for } k = 0, 1, 2, \ldots$$  

(2.1)

By rewriting the inequality (2.1) in terms of the two-point distance distribution, we have the following theorem.
Theorem 2.1. For a spherical set $X$ in $\mathbb{S}^{d-1}$ with inner product set $A$, $\sum_{t \in A} x(t) = N(N-1)$ and
\[ N + \sum_{t \in A} x(t) P_k^d(t) \geq 0 \text{ for } k \geq 1. \]

Part 4. One can establish a linear program using Theorem 2.1 to bound the cardinality $N$.

2.2 Three-point semidefinite constraint

Part 1. Consider the three-point distance distribution
\[ y(u, v, t) := \# \{(b, c, c') \in X^3 : b \cdot c = u, b \cdot c' = v, c \cdot c' = t\}. \]
The value $y(u, v, t)$ counts the number of triples in $X$ with pairwise inner products $u$, $v$ and $t$.

Part 2. The distance distributions are related to each other and the cardinality $N$ by
- $y(1, 1, 1) = x(1) = N$,
- $y(1, t, t) = y(t, 1, t) = y(t, t, 1) = x(t)$,
- $y(1, u, v) = y(u, 1, v) = y(u, v, 1) = 0$ for $u \neq v$, and
- $\sum_{u, v, t \in A} y(u, v, t) = N(N-1)(N-2)$.

Part 3. Bachoc and Vallentin [3] proved that, there is a specific series of matrices $\{Y_{k,n}^d : k \geq 0, n \geq 0\}$ such that
\[ \sum_{c, c' \in X} Y_{k,n}^d (b \cdot c, b \cdot c', c \cdot c') \succeq 0 \] (2.2)
for any fixed point $b \in \mathbb{S}^{d-1}$. The matrices $Y_{k,n}^d$ are defined by
\[ Y_{k,n}^d (u, v, t) := Q_k^d (u, v, t) \begin{pmatrix} 1 \\ u \\ \vdots \\ u^n \end{pmatrix} \begin{pmatrix} 1 & v & \cdots & v^n \end{pmatrix}, \]
\[ Q_k^d (u, v, t) := (1 - u^2)^{k/2} (1 - v^2)^{k/2} P_k^{d-1} \left( \frac{t - uv}{\sqrt{(1 - u^2)(1 - v^2)}} \right). \]
The order of $Y_{k,n}^d (u, v, t)$ is $n + 1$, and in which every entry is a polynomial of $u, v, t$ in degree $k$.

By summing $b$ in (2.2) over elements of $X$, we have the following constraints about $y(u, v, t)$.

Theorem 2.2 (Bachoc and Vallentin [3]). For a spherical set $X$ in $\mathbb{S}^{d-1}$ with inner product set $A$,
\[ \sum_{u, v, t \in A} y(u, v, t) = (N-2) \sum_{t \in A} x(t) \]
and
\[ NY_{k,n}^d (1, 1, 1) + \sum_{t \in A} x(t) \left( Y_{k,n}^d (1, t, t) + Y_{k,n}^d (t, 1, t) + Y_{k,n}^d (t, t, 1) \right) + \sum_{u, v, t \in A} y(u, v, t) Y_{k,n}^d (u, v, t) \geq 0 \text{ for } k, n \geq 0. \]
The positive semidefiniteness means that $Q$ is positive semidefinite. We denote the matrix (2.4) by $Q_k^d$, and the objective function is $1 + \sum_t x(t)/N = N$.

Below shows an alternative version of Theorem 2.2.

**Part 3 (alternative version).** Let $A' = A \cup \{1\}$. The semidefinite constraint in Theorem 2.2 is equivalent to

$$\sum_{u,v,t \in A'} y(u,v,t)Q_k^d(u,v,t) \begin{pmatrix} 1 \\ u \\ \vdots \\ u^n \end{pmatrix} \begin{pmatrix} 1 & v & \cdots & v^n \end{pmatrix} \geq 0.$$  

The positive semidefiniteness means that

$$a^\top \left( \sum_{u,v,t \in A'} y(u,v,t)Q_k^d(u,v,t) \begin{pmatrix} 1 \\ u \\ \vdots \\ u^n \end{pmatrix} \begin{pmatrix} 1 & v & \cdots & v^n \end{pmatrix} \right) a \geq 0$$

for all $a \in \mathbb{R}^{n+1}$, or

$$\sum_{u,v,t \in A'} y(u,v,t)Q_k^d(u,v,t)f(u)f(v) \geq 0 \quad (2.3)$$

for all polynomials $f(x)$ with degree at most $n$. Since $n$ can be arbitrary, the inequality (2.3) holds for any polynomial $f(x)$.

Let $\{e_u : u \in A'\}$ be the standard basis of $\mathbb{R}^{n+1}$. We rewrite (2.3) as

$$\sum_{u,v,t \in A'} y(u,v,t)Q_k^d(u,v,t)(f^\top e_u)(e_v^\top f) \geq 0$$

where $f = \sum_{u \in A'} f(u)e_u$ for some polynomial $f(x)$. In fact, $f$ can be taken as arbitrary vector in $\mathbb{R}^{n+1}$; that is, given any vector $f = \sum_{u \in A'} f_u e_u$, we can always find a polynomial $f(x)$ such that $f(u) = f_u$, $u \in A'$.

Therefore, the matrix

$$\sum_{u,v,t \in A'} y(u,v,t)Q_k^d(u,v,t)e_u e_v^\top$$

is positive semidefinite. We denote the matrix (2.4) by $Q_k^d(X)$, and call it by the **alternative three-point semidefinite constraint**.

**Theorem 2.3 (Alternative three-point semidefinite constraint).** For a spherical $s$-distance set $X$ in $S^{d-1}$ with inner product set $A$,

$$\sum_{u,v,t \in A} y(u,v,t) = (N-2) \sum_{t \in A} x(t).$$

Let $\{e_u : u \in A \cup \{1\}\}$ be the standard basis of $\mathbb{R}^{n+1}$. Then

$$Q_k^d(X) = NQ_k^d(1,1,1)e_1 e_1^\top + \sum_{t \in A} x(t) \left( Q_k^d(1,1,t)e_1 e_t^\top + Q_k^d(1,t,1)e_1 e_t^\top + Q_k^d(t,1,1)e_t e_1^\top \right) + \sum_{u,v,t \in A} y(u,v,t)e_u e_v^\top \geq 0$$
Remark 2.4. When the concerned object $X$ has a finite number of distances, the alternative semidefinite constraints $Q^d_k(X)$ are simpler than the original ones in Theorem 2.2. For a spherical $s$-distance set $X$, the original constraints consist of sums of $s^3 + 3s + 1$ matrices with order $(n + 1)$; in the alternative constraints $Q^d_k(X)$, there are only $s^3 + 3s + 1$ terms in a $(s + 1) \times (s + 1)$ matrix.

Remark 2.5. One might think that the original semidefinite constraints are better with larger matrix size $(n + 1)$. However, an argument similar to the proof of Theorem 2.3 indicates that the restricting ability on $y(u,v,t)$ of the original semidefinite constraints is the same as the alternative constraints whenever $n \geq s$. Therefore, it suffices to take $n = s$ when applying the original semidefinite constraints.

Example 2.6. Consider a 2-distance set $X$ with $A(X) = \{\alpha, \beta\}$. The alternative three-point semidefinite constraint is

$$Q^d_k(X) = \begin{pmatrix}
NQ^d_k(1,1,1) & x(\alpha)Q^d_k(1,\alpha,\alpha) & x(\beta)Q^d_k(1,\beta,\beta) \\
x(\alpha)Q^d_k(\alpha,1,\alpha) & y(\alpha,\alpha,\alpha)Q^d_k(\alpha,\alpha,\alpha) & y(\alpha,\alpha,\beta)Q^d_k(\alpha,\alpha,\beta) \\
x(\beta)Q^d_k(\beta,1,\beta) & y(\beta,\alpha,\alpha)Q^d_k(\beta,\alpha,\alpha) & y(\beta,\beta,\beta)Q^d_k(\beta,\beta,\beta)
\end{pmatrix} \succeq 0.$$

2.3 Multi-point semidefinite constraint

The multi-point semidefinite constraints are generalizations of the three-point semidefinite constraints. Fix $m$ to be a positive integer with $1 \leq m \leq d - 2$. The multi-point constraints become the three-point constraints when $m = 1$.

Part 1. We use the notation of Gram matrices to define the multi-point distance distribution.

Definition 2.7. Suppose $B = \{b_1, \ldots, b_m\} \subseteq X$ is a set of unit vectors, and $c, c' \in S^{d-1}$.

(a) The Gram matrix of $B$ is an $m \times m$ matrix

$$G = G(B) := (b_p \cdot b_q)_{1 \leq p,q \leq m}.$$

The Gram matrix $G$ is symmetric and positive semidefinite. If $G$ is positive definite, i.e., $B$ is linearly independent, we say $G$ is a proper Gram matrix.

(b) For $c \in S^{d-1}$, denote the vector $B^T \cdot c := (b_1 \cdot c, \ldots, b_m \cdot c)^T$ in $\mathbb{R}^m$.

(c) Suppose $u = B^T \cdot c \in \mathbb{R}^m$, then the Gram matrix of $B \cup \{c\}$ is

$$G(B,c) = \begin{pmatrix}
G(B) & B^T \cdot c \\
(c^T \cdot B & c \cdot c)
\end{pmatrix} = \begin{pmatrix}
G & u^T \\
u & 1
\end{pmatrix}.$$

We denote the $(m + 1) \times (m + 1)$ Gram matrix by the pair $(G; u)$.

(d) Suppose $u = B^T \cdot c$ and $v = B^T \cdot c'$, then the Gram matrix of $B \cup \{c, c'\}$ is

$$G(B,c,c') = \begin{pmatrix}
G(B) & B^T \cdot c & B^T \cdot c' \\
(c^T \cdot B & c \cdot c & c \cdot c' \\
(c' \cdot B & c' \cdot c & c' \cdot c')
\end{pmatrix} = \begin{pmatrix}
G & u & v \\
u^T & 1 & t \\
v & t & 1
\end{pmatrix}.$$
We denote the \((m + 2) \times (m + 2)\) Gram matrix by the tuple \((G; \mathbf{u}, \mathbf{v}, t)\).

**Definition 2.8.** Suppose \(G\) is an \(m \times m\) proper Gram matrix, \(\mathbf{u}, \mathbf{v} \in \mathbb{R}^m\) and \(t \in \mathbb{R}\). Define the \((m + 2)\)-point distance distribution by

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) := \#\{(B, c, c') \in X^{m+2} : G(B, c, c') = (G; \mathbf{u}, \mathbf{v}, t)\},
\]

that is, the number of \((m + 2)\)-tuples \((B, c, c')\) with a specific Gram matrix. Also, we can define the \((m + 1)\)-point and \(m\)-point distance distributions

\[
N_{m-1}(G; \mathbf{u}) := \#\{(B, c) \in X^{m+1} : G(B, c) = (G; \mathbf{u})\},
\]

\[
N_{m-2}(G) := \#\{B \in X^m : G(B) = G\}.
\]

**Remark 2.9.** For \(m = 1\), \(G = (1)\) and \(N_1(G; \mathbf{u}, \mathbf{v}, t)\) is the three-point distance distribution \(y(u, v, t)\); for \(m = 0\), \((m + 2)\)-tuples \((B, c, c')\) degenerated to pairs, so \(N_0(G)\) is the two-point distance distribution \(x(t)\) if \(G = \begin{pmatrix} 1 & t \\ t & 1 \end{pmatrix}\); for \(N = -1\), define \(N_{-1} = N\).

**Part 2.** The distance distribution \(N_m\) is related to the cardinality \(N\) by the following equation:

\[
\sum_{G} \sum_{\mathbf{u}, \mathbf{v} \in A(X)^m} \sum_{t \in A(X)} N_m(G; \mathbf{u}, \mathbf{v}, t) = \frac{N!}{(N - m - 2)!},
\]

in which \(G\) is summed over all possible \(m \times m\) proper Gram matrices. Furthermore, we have the following relations for \(N_m\) and their degenerations.

**Proposition 2.10.** Let \(G\) be an \(m \times m\) proper Gram matrix and \(N_m\) be defined as above. Let \(G_{(p)}\) be the \(p\)-th column of \(G\).

(a) Suppose \(u_p = v_q = 1\) for some \(1 \leq p, q \leq m\). Then

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) = \begin{cases} N_{m-2}(G) & \text{if } \mathbf{u} = G_{(p)}, \mathbf{v} = G_{(q)}, t = g_{pq}, \\ 0 & \text{otherwise}. \end{cases}
\]

(b) Suppose \(u_p = 1\) for some \(1 \leq p \leq m\). Then

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) = \begin{cases} N_{m-1}(G; \mathbf{v}) & \text{if } \mathbf{u} = G_{(p)}, t = v_p, \\ 0 & \text{otherwise}. \end{cases}
\]

Similarly, suppose \(v_q = 1\) for some \(1 \leq q \leq m\). Then

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) = \begin{cases} N_{m-1}(G; \mathbf{u}) & \text{if } \mathbf{v} = G_{(q)}, t = u_q, \\ 0 & \text{otherwise}. \end{cases}
\]

(c) Suppose \(t = 1\). Then

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) = \begin{cases} N_{m-1}(G; \mathbf{u}) & \text{if } \mathbf{u} = v, \\ 0 & \text{otherwise}. \end{cases}
\]

**Proof.** For (a), recall that \(N_m(G; \mathbf{u}, \mathbf{v}, t)\) counts the tuples \((B, c, c')\) with

\[
b_p \cdot b_q = g_{pq}, \ b_p \cdot c = u_p, \ b_q \cdot c' = v_q, \ c \cdot c' = t.
\]
If \( u_p = v_q = 1 \), then \( c = b_p \) and \( c' = b_q \). Therefore, the \((m + 1)\)-th column and the \(p\)-th column in \((G; u, v, t)\) must be the same, i.e., \( u = G(p) \) and \( t = v_p \). Similarly, \( v = G(q) \) and \( t = u_q = G_pq \).

Hence \( N_m(G; u, v, t) > 0 \) only if \( u = G(p) \), \( v = G(q) \) and \( t = G_pq \); also, the Gram matrix \((G; u, v, t)\) of \((B, c, c')\) degenerates to the Gram matrix \( G\) of \( B\).

For (b), if \( u_p = 1 \) then \( c = b_p \), and the Gram matrix of \((B, c, c')\) degenerates to that of \((B, c')\); if \( v_q = 1 \) then \( c' = b_p' \), and the Gram matrix degenerates to that of \((B, c)\). For (c), if \( t = 1 \) then \( c = c' \), and the Gram matrix degenerates to that of \((B, c)\).

\(\Box\)

**Part 3.** Musin [32] proved a multi-point generalization for the semidefinite constraints (2.2), which we use to formulate the constraints for the multi-point distance distribution \( N_m \).

**Definition 2.11 (Musin [32]).** Let \( G \) be an \( m \times m \) proper Gram matrix, \( u, v \in \mathbb{R}^m \) and \( t \in \mathbb{R} \).

Define the *multivariate Gegenbauer polynomials* by

\[
Q_{k}^{d,m}(G; u, v, t) := (1 - uG^{-1}u^\top)^{k/2}(1 - vG^{-1}v^\top)^{k/2}P_k^{d-m}\left(\frac{t - uG^{-1}v^\top}{\sqrt{(1 - uG^{-1}u^\top)(1 - vG^{-1}v^\top)}}\right).
\]

Let \( B_n(u) \) be the column vector collecting all monomials of \( \{u_1, \ldots, u_m\} \) with degree at most \( n \). Define the matrices \( Y_{k,n}^{d,m}(G; u, v, t) \) by

\[
Y_{k,n}^{d,m}(G; u, v, t) := Q_{k}^{d,m}(G; u, v, t)B_n(u)B_n(v)^\top.
\]

The order of \( Y_{k,n}^{d,m} \) is \( \binom{n+m}{m} \), and in which every entry is a polynomial of \( u, v, t \) in degree \( k \). When \( m = 1 \), the Gram matrix \( G \) is the identity matrix of order 1, and the above definitions of \( Q_{k}^{d,m} \) and \( Y_{k,n}^{d,m} \) agree with \( Q_k^d \) and \( Y_{k,n}^{d} \) defined by Bachoc and Vallentin [3].

Fix a subset \( B = \{b_1, \ldots, b_m\} \subseteq X \) of linearly independent vectors. Let \( G = G(B) \) be the Gram matrix of \( B \). Musin [32] proved that

\[
\sum_{c, c' \in X} Y_{k,n}^{d,m}(G; B^\top \cdot c, B^\top \cdot c', c \cdot c') \geq 0. \tag{2.5}
\]

By summing \( B \) in (2.5) over all subsets of \( X \) with fixed proper Gram matrix \( G \), we have the following constraints about \( N_m \).

**Theorem 2.12.** For a spherical set \( X \) in \( S^{d-1} \) with inner product set \( A \),

\[
\sum_G \sum_{u,v \in A^m} \sum_{t \in A} N_m(G; u, v, t) = \frac{N!}{(N - m - 2)!},
\]

in which \( G \) is summed over all possible \( m \times m \) proper Gram matrices. Let \( A' = A \cup \{1\} \). For a fixed \( m \times m \) proper Gram matrix \( G \),

\[
\sum_{u,v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t) Y_{k,n}^{d,m}(G; u, v, t) \geq 0 \text{ for } k, n \geq 0.
\]

Note that there is one semidefinite constraint for each proper Gram matrix \( G \). For example, for a spherical \( s \)-distance set \( X \) with \( -1 \notin A(X) \), there are \( s \) possible \( 2 \times 2 \) proper Gram matrices \( G \), and accordingly \( s \) different semidefinite constraints for the 4-point distance distribution \( N_2(G; u, v, t) \).

**Part 3 (alternative version).** Similar to the relation of Theorem 2.2 and Theorem 2.3 there is also an alternative version of Theorem 2.12. We call it the **alternative multi-point semidefinite constraint**.
Theorem 2.13 (Alternative multi-point semidefinite constraint). For a spherical $s$-distance set $X$ in $\mathbb{S}^{d-1}$ with inner product set $A$,
\[ \sum_{G} \sum_{u, v \in A^m} \sum_{t \in A} N_m(G; u, v, t) = \frac{N!}{(N - m - 2)!}, \]
in which $G$ is summed over all possible $m \times m$ proper Gram matrices. Let $A' = A \cup \{1\}$ and \{e_u : u \in (A')^m\} be the standard basis of $\mathbb{R}^{(s+1)^m}$. Then for a fixed $m \times m$ proper Gram matrix $G$,
\[ Q_k^{d,m}(G; X) := \sum_{u, v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t)Q_k^{d,m}(G; u, v, t)e_u e_v^\top \geq 0 \text{ for } k \geq 0. \]

Proof. The proof is similar to the proof of Theorem 2.12. By Theorem 2.12
\[ \sum_{u, v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t)Y_{k,n}(G; u, v, t) \geq 0, \]
i.e.,
\[ \sum_{u, v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t)Q_k^{d,m}(G; u, v, t)B_n(u)B_n(v)^\top \geq 0. \]
Hence
\[ \sum_{u, v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t)Q_k^{d,m}(G; u, v, t)f(u)f(v) \geq 0 \quad (2.6) \]
for all $m$-variable polynomials $f$, since the degree $n$ is arbitrary.

Let $f = \sum_{u \in (A')^m} f(u)e_u \in \mathbb{R}^{(m+1)^r}$. Then inequality (2.6) becomes
\[ f^\top \left( \sum_{u, v \in (A')^m} \sum_{t \in A'} N_m(G; u, v, t)Q_k^{d,m}(G; u, v, t)e_u e_v^\top \right) f = f^\top Q_k^{d,m}(G; X)f \geq 0 \]
for all possible $f$. Since the possible range of $f$ is as large as $\mathbb{R}^{(m+1)^r}$, $Q_k^{d,m}(G; X)$ is positive semidefinite. \hfill \Box

For a spherical $s$-distance set $X$, the matrices $Q_k^{d,m}(G; X)$ in the above semidefinite constraints are $(s+1)^m \times (s+1)^m$ matrices, in which every entry contains $(s+1)$ terms corresponding to $(s+1)$ values $t \in A'$. When $k = 0$, the polynomial $Q_k^{d,m}$ is constant; when $k > 0$, the polynomial $Q_k^{d,m}(G; u, v, t)$ vanishes for some specific input. In either case, the matrix $Q_k^{d,m}(G; X)$ has a cleaner format. As the following indicates, $Q_k^{d,m}(G; X)$ can be represented as a $(s^m + 1) \times (s^m + 1)$ matrix if $k = 0$, and a $s^m \times s^m$ matrix if $k \geq 1$.

Corollary 2.14. Let $G_{(p)}$ be the $p$-th column of $G$.

(a) For $k = 0$, let $e_1 = e_G^{(1)} + \cdots + e_G^{(m)}$. Then
\[ Q_0^{d,m}(G; X) = N_{m-2}(G)e_1 e_1^\top + \sum_{u \in A^m} N_{m-1}(G; u)(e_1 e_u^\top + e_u e_1^\top + e_u e_u^\top) + \sum_{u, v \in A^m} \sum_{t \in A} N_m(G; u, v, t)e_u e_v^\top. \]
(b) For \( k \geq 1 \),
\[
Q_{k}^{d,m}(G; X) = \sum_{u \in A^{m}} N_{m-1}(G; u)Q_{k}^{d,m}(G; u, u, 1)e_u e_u^T \\
+ \sum_{u,v \in A^m} \sum_{t \in A} N_m(G; u, v, t)Q_{k}^{d,m}(G; u, v, t)e_u e_v^T.
\]

Proof. By Proposition 2.10 if at least one of \( \{u_1, \ldots, u_m, v_1, \ldots, v_m\} \) equals 1, then there is at most one \( N_m(G; u, v, t) \) being positive among all \( t \in A' \); if \( t = 1 \), then \( N_m(G; u, v, t) > 0 \) only when \( u = v \). After specifying all the special cases, the matrix \( Q_{k}^{d,m}(G; X) \) becomes
\[
Q_{k}^{d,m}(G; X) = \sum_{1 \leq p, q \leq m} N_{m-2}(G)Q_{k}^{d,m}(G; G(p), G(q), G_{pq})e_{G(p)} e_{G(q)}^T \\
+ \sum_{1 \leq p \leq m, v \in A^m} N_{m-1}(G; v)Q_{k}^{d,m}(G; G(p), v, v_p)e_{G(p)} e_{v_p}^T \\
+ \sum_{u \in A^m} N_{m-1}(G; u)Q_{k}^{d,m}(G; u, G(q), u_q)e_{u} e_{G(q)}^T \\
+ \sum_{u \in A^m} N_{m-1}(G; u)Q_{k}^{d,m}(G; u, u, 1)e_{u} e_{u}^T \\
+ \sum_{u, v \in A^m} \sum_{t \in A} N_m(G; u, v, t)Q_{k}^{d,m}(G; u, v, t)e_u e_v^T.
\]

The equation in (a) follows from the fact that \( Q_{k}^{d,m}(G; u, v, t) \equiv 1 \). For (b), we claim that all \( Q_{k}^{d,m}(G; u, v, t) \) in the first three lines vanish since \( Q_{k}^{d,m}(G; u, v, t) \) is a polynomial in \( t - uG^{-1}v^T \) and \( (1 - uG^{-1}u^T)(1 - vG^{-1}v^T) \). For example, with input \( G; u, v, t \) = \( (G; G(p), v, v_p) \) in the second line,
\[
t - uG^{-1}v^T = v_p - G(p)^{-1}G(p)^T = v_p - e_p v^T = v_p - v_p = 0
\]
and
\[
1 - uG^{-1}u^T = 1 - G(p)^{-1}G(p)^T = 1 - G_{pp} = 0,
\]
so \( Q_{k}^{d,m}(G; G(p), v, v_p) = 0 \).

Part 4. One can establish a semidefinite program using Theorem 2.12 or using Theorem 2.13 to bound the cardinality \( N \).

3 Switching reduction

In this section, we give a simplification of the semidefinite constraints on the regime that \( X \) is a spherical projection of a set of equiangular lines, which we call by switching reduction.

The simplification is given by considering the mutual relations of different spherical projections. We say that two Gram matrices \( G_1, G_2 \) are switching equivalent, if \( G_2 \) is given by changing the sign of some columns and the corresponding rows in \( G_1 \). The Gram matrices of different spherical projections of the same set of equiangular lines are switching equivalent: let \( X = \{c_1, \ldots, c_N\} \) be a spherical projection with Gram matrix \( G = G(X) \). Any possible spherical projection is of the form
\[
\{\varepsilon_1 c_1, \ldots, \varepsilon_N c_N\}, \varepsilon_i \in \{\pm 1\}.
\]
Let $\Lambda = \text{diag}(\varepsilon_1, \ldots, \varepsilon_N)$ be the diagonal matrix with diagonal entries $\varepsilon_1, \ldots, \varepsilon_N$. Then the Gram matrix $G_A$ of the corresponding spherical projection is

$$G_A = (\varepsilon_i \varepsilon_j)^{1 \leq i, j \leq N} = \Lambda A.$$

That is, $G_A$ is given by changing the sign of the column $i$ and the corresponding row $i$ with $\varepsilon_i = -1$. Then $G_A$ is switching equivalent to $G$.

In the following, we demonstrate the modification of the semidefinite constraints after switching reduction.

**Part 1.** We can define the distance distribution $N_m(G; u, v, t)$ for a spherical projection $X$ of a set of equiangular lines. Meanwhile, we can never define $N_m(G; u, v, t)$ for the set of equiangular lines itself, since the number of $(m+2)$-tuples with a fixed Gram matrix depends on the chosen spherical projection. However, the sum of $N_m(G; u, v, t)$ over a switching class of the Gram matrix $(G; u, v, t)$ is independent of the choice of spherical projections.

We define the **distance distribution of switching classes**, which do not rely on the spherical projections. We use square brackets to represent the sums over switching classes.

**Definition 3.1.** Suppose $G$ is an $m \times m$ proper Gram matrix and $u_i, v_j, t \in \{\pm \alpha\}$. Define the distance distribution of the switching class $[G; u, v, t]$ by

$$N_m[G; u, v, t] := \sum_{(G'; u', v', t') \sim (G; u, v, t)} N_m(G'; u', v', t'),$$

in which $\sim$ means switching equivalence. The value $N_m[G; u, v, t]$ is the number of $(m+2)$-tuples $(B, c, c')$ with Gram matrix switching equivalent to $(G; u, v, t)$. We also define

$$N_{m-1}[G; u] = \sum_{(G'; u') \sim (G; u)} N_{m-1}(G'; u'),$$

$$N_{m-2}[G] = \sum_{G' \sim G} N_{m-2}(G').$$

Algebraically, $(G'; u', v', t')$ is switching equivalent to $(G; u, v, t)$ if and only if

$$(G'; u', v', t') = \Lambda_0(G; u, v, t)\Lambda_0$$

for some $(m+2)\times(m+2)$ diagonal matrix $\Lambda_0 = \text{diag}(\varepsilon_1, \ldots, \varepsilon_{m+2})$ with diagonal entries $\varepsilon_1, \ldots, \varepsilon_{m+2} \in \{\pm 1\}$. Write $\Lambda = \text{diag}(\varepsilon_1, \ldots, \varepsilon_m)$, we have

$$\begin{pmatrix} G' & u' & v' \\ (u')^T & 1 & t' \\ (v')^T & t' & 1 \end{pmatrix} = \begin{pmatrix} \Lambda & 0 & 0 \\ 0 & \varepsilon_{m+1} & 0 \\ 0 & 0 & \varepsilon_{m+2} \end{pmatrix} \begin{pmatrix} G & u & v \\ (u^T) & 1 & t \\ (v^T) & t & 1 \end{pmatrix} \begin{pmatrix} \Lambda & 0 & 0 \\ 0 & \varepsilon_{m+1} & 0 \\ 0 & 0 & \varepsilon_{m+2} \end{pmatrix},$$

therefore

$$G' = \Lambda \Lambda G, \quad u' = \varepsilon_{m+1}Au, \quad v' = \varepsilon_{m+2}Av, \quad t' = \varepsilon_{m+1}\varepsilon_{m+2}t.$$

**Proposition 3.2.** Let $G$ be an $m \times m$ proper Gram matrix and $u_i, v_j, t \in \{\pm \alpha\}$. Then

(a) $N_m[G; u, v, t] = \frac{1}{2} \sum_\Lambda \sum_{\varepsilon_{m+1}, \varepsilon_{m+2} \in \{\pm 1\}} N_m(\Lambda \Lambda G; \varepsilon_{m+1}Au, \varepsilon_{m+2}Av, \varepsilon_{m+1}\varepsilon_{m+2}t).$
Let Proposition 3.3. 

\[ N_{m-1}[G; \mathbf{u}] = \frac{1}{2} \sum \sum_{\varepsilon_{m+1} \in \{\pm 1\}} N_{m-1}(AGA; \varepsilon_{m+1} \mathbf{u}). \]

(c) \[ N_{m-2}[G] = \frac{1}{2} \sum \sum N_{m-2}(AGA). \]

In all cases, \( \Lambda \) is summed over all \( m \times m \) diagonal matrices with diagonal entries \( \varepsilon_1, \ldots, \varepsilon_m \in \{\pm 1\} \).

There is a multiple 1/2 in Proposition 3.2 since two diagonal matrices define the same Gram matrix if and only if the matrices are opposite.

**Part 2.** The distance distribution \( N_m[G; \mathbf{u}, \mathbf{v}, t] \) of switching classes are related to the cardinality \( N \) by the following equations.

**Proposition 3.3.** Let \( \mathcal{G} \) be a collection of representatives of switching classes of \( m \times m \) proper Gram matrices. Fix \( u_1 = v_1 = \alpha \), and let \( u_p, v_q, t \in \{\pm \alpha\} \) for \( 2 \leq p, q \leq m \). Then

\[
\sum_{G \in \mathcal{G}} u_1 = v_1 = \alpha \sum_{t \in \{\pm \alpha\}} N_m[G; \mathbf{u}, \mathbf{v}, t] = \frac{N!}{(N-m-2)!},
\]

\[
\sum_{G \in \mathcal{G}} u_1 = \alpha \sum N_m-1[G; \mathbf{u}] = \frac{N!}{(N-m-1)!},
\]

\[
\sum_{G \in \mathcal{G}} N_{m-2}[G] = \frac{N!}{(N-m)!}.
\]

**Proof.** The right hand side of the first equation is the sum of \( N_m(G; \mathbf{u}, \mathbf{v}, t) \) over all proper \( (m+2) \times (m+2) \) Gram matrices \( N_m(G; \mathbf{u}, \mathbf{v}, t) \). For any \( (G'; \mathbf{u}', \mathbf{v}', t') \), there is exactly one \( m \times m \) Gram matrix \( G = AG'A \) which is switching equivalent to \( G' \). Therefore, the number \( N_m(G'; \mathbf{u}', \mathbf{v}', t') \) is counted in

\[
N_m[G; \varepsilon \Lambda \mathbf{u}', \varepsilon' \Lambda \mathbf{v}', \varepsilon \varepsilon' t']
\]

for \( \varepsilon, \varepsilon' \in \{\pm 1\} \). Only one of the four terms is counted in the left hand side since \( u_1 \) and \( v_1 \) are restricted to \(+\alpha\). Therefore, the both sides are the same. By similar arguments the other two equations are true.

There are several duplications of values in the distance distribution \( N_m(G; \mathbf{u}, \mathbf{v}, t) \), as

\[
N_m(G; \mathbf{u}, \mathbf{v}, t) = N_m(G'; \mathbf{u}', \mathbf{v}', t')
\]

if the matrices \( (G; \mathbf{u}, \mathbf{v}, t) \), \( (G'; \mathbf{u}', \mathbf{v}', t') \) are identical up to permutations. We extend this fact to the duplication of values in the distance distribution of switching classes.

**Proposition 3.4.** If \( (G'; \mathbf{u}', \mathbf{v}', t') \) is switching equivalent to \( P(G; \mathbf{u}, \mathbf{v}, t)P^T \) for some permutation matrix \( P \), then \( N_m[G'; \mathbf{u}', \mathbf{v}', t'] = N_m[G; \mathbf{u}, \mathbf{v}, t] \). Similarly, if \( (G'; \mathbf{u}') \) is switching equivalent to \( P(G; \mathbf{u})P^T \) for some permutation matrix \( P \), then \( N_{m-1}[G'; \mathbf{u}] = N_{m-1}[G; \mathbf{u}] \): if \( G' \) is switching equivalent to \( PGP^T \) for some permutation matrix \( P \), then \( N_{m-2}[G'] = N_{m-2}[G] \).

**Example 3.5.** For the two-point distance distribution, the two \( 2 \times 2 \) proper Gram matrices are switching equivalent to each other, so \( N_0[G] = N(N-1) \) for either \( G \). For the three-point distance distribution, note that any \( 3 \times 3 \) proper Gram matrix \( (1; u, v, t) \) is switching equivalent to either

\[
\begin{pmatrix}
1 & \alpha & \alpha \\
\alpha & 1 & \alpha \\
\alpha & \alpha & 1
\end{pmatrix}
\]

or

\[
\begin{pmatrix}
1 & \alpha & \alpha \\
\alpha & 1 & -\alpha \\
\alpha & -\alpha & 1
\end{pmatrix},
\]

so there are 2 switching classes in total. Denote

\[
y_1 := N_1[1; \alpha, \alpha, \alpha] = y(\alpha, \alpha, \alpha) + y(\alpha, -\alpha, -\alpha) + y(-\alpha, \alpha, -\alpha) + y(-\alpha, -\alpha, \alpha),
\]

\[
y_2 := N_1[1; \alpha, \alpha, -\alpha] = y(\alpha, \alpha, -\alpha) + y(\alpha, -\alpha, \alpha) + y(-\alpha, \alpha, \alpha) + y(-\alpha, -\alpha, -\alpha).
\]
By Proposition 3.3, \( y_1 + y_2 = N!/(N-3)! = N(N-1)(N-2) \). For the four-point distance distribution \( N_2[G; \mathbf{u}, \mathbf{v}, t] \), note that any \( 4 \times 4 \) proper Gram matrix \( (G'; \mathbf{u}', \mathbf{v}', t') \) is switching equivalent to a Gram matrix of the form
\[
\begin{pmatrix}
G & \mathbf{u} & \mathbf{v} \\
\mathbf{u}^\top & 1 & t \\
\mathbf{v}^\top & t & 1
\end{pmatrix} = \begin{pmatrix}
1 & \alpha & \alpha & \alpha \\
\alpha & 1 & \mathbf{u}_2 & \mathbf{v}_2 \\
\alpha & \mathbf{u}_2 & 1 & t \\
\alpha & \mathbf{v}_2 & t & 1
\end{pmatrix},
\]
so there are \( 2^d = 8 \) switching classes in total. Furthermore, the six Gram matrices
\[
\begin{pmatrix}
1 & \alpha & \alpha & \alpha \\
\alpha & 1 & \alpha & -\alpha \\
\alpha & \alpha & 1 & -\alpha \\
\alpha & -\alpha & 1 & 1
\end{pmatrix},
\]
are identical up to switching and permutations. Let \( \mathbf{u}_1 = (\alpha \ -\alpha)^\top \) and \( \mathbf{u}_2 = (\alpha \ -\alpha)^\top \). By Proposition 3.3
\[
N_2[G; \mathbf{u}_1, \mathbf{u}_1, -\alpha] = N_2[G; \mathbf{u}_1, \mathbf{u}_2, \alpha] = N_2[G; \mathbf{u}_1, \mathbf{u}_2, -\alpha] = N_2[G; \mathbf{u}_2, \mathbf{u}_1, \alpha] = N_2[G; \mathbf{u}_2, \mathbf{u}_2, -\alpha].
\]
Denote \( z_1 := N_2[G; \mathbf{u}_1, \mathbf{u}_1, \alpha] \), \( z_2 := N_2[G; \mathbf{u}_1, \mathbf{u}_1, -\alpha] \) and \( z_3 := N_2[G; \mathbf{u}_2, \mathbf{u}_2, -\alpha] \). By Proposition 3.3 we have \( z_1 + 6z_2 + 3z_3 = N(N-1)(N-2)(N-3) \).

Remark 3.6. In general, there are \( 2^{(m+2)} \) different \((m+2) \times (m+2)\) Gram matrices and \( 2^{(m+1)} \) switching classes. In the spirit of Proposition 3.3 there are at most \( a(m+2) \) different values of the distance distribution \( N_m[G; \mathbf{u}, \mathbf{v}, t] \) of switching classes, where \( a(m) \) is the number of Seidel matrices of order \( m \). The first seven terms for \( a(m) \) is 1, 1, 2, 3, 7, 16, 54; see Sequence A002854 in The On-Line Encyclopedia of Integer Sequences [38] for detail. Therefore, the number of variables of a semidefinite program developed by \((m+2)\)-point semidefinite constraints is decreased to \( a(m+2) \) after switching reduction.

Part 3. The reduction in the alternative semidefinite constraints \( Q_k^{d,m}(G; X) \) is due to the switching property of the polynomial \( Q_k^{d,m}(G; \mathbf{u}, \mathbf{v}, t) \).

Proposition 3.7. If \((G'; \mathbf{u}', \mathbf{v}', t)\) is switching equivalent to \((G; \mathbf{u}, \mathbf{v}, t)\) by the relation
\[
G' = \Lambda G \Lambda, \quad \mathbf{u}' = \varepsilon_{m+1} \Lambda \mathbf{u}, \quad \mathbf{v}' = \varepsilon_{m+2} \Lambda \mathbf{v}, \quad t' = \varepsilon_{m+1} \varepsilon_{m+2} t,
\]
then \( Q_k^{d,m}(G'; \mathbf{u}', \mathbf{v}', t') = (\varepsilon_{m+1} \varepsilon_{m+2})^{k} Q_k^{d,m}(G; \mathbf{u}, \mathbf{v}, t) \) for any \( k \geq 0 \).

Proof. Since
\[
t' - \mathbf{u}'(G')^{-1}(\mathbf{v}')^\top = \varepsilon_{m+1} \varepsilon_{m+2} (t - \mathbf{u} G^{-1} \mathbf{v}^\top)
\]
and
\[
(1 - \mathbf{u}'(G')^{-1}(\mathbf{u}')^\top)(1 - \mathbf{v}'(G')^{-1}(\mathbf{v}')^\top) = (1 - \mathbf{u} G^{-1} \mathbf{u}^\top)(1 - \mathbf{v} G^{-1} \mathbf{v}^\top),
\]
the only difference in \( Q_k^{d,m}(G; \mathbf{u}, \mathbf{v}, t) \) and \( Q_k^{d,m}(G'; \mathbf{u}', \mathbf{v}', t') \) is the input of \( P_k^{d,m} \) in a multiple \( \varepsilon_{m+1} \varepsilon_{m+2} \). Meanwhile, \( P_k^{d,m} \) is an odd function when \( k \) is odd and an even function when \( k \) is even, so the two values differ by a multiple of \( (\varepsilon_{m+1} \varepsilon_{m+2})^k \).
Due to Proposition 3.7, we can safely sum over switching classes in the alternative semidefinite constraints $Q^d_m(G; X)$, since the coefficients $Q^d_m$ for inputs $(G; u, v, t)$ in the same switching class are identical. We also use the square bracket to represent the sum of the matrices over a switching class.

**Theorem 3.8.** For a spherical projection $X$ of a set of equiangular lines in $\mathbb{R}^d$ with inner product set $A = \{ \pm \alpha \}$, fix $u_1, v_1 = \alpha$, and let $u_p, v_q, t \in \{ \pm \alpha \}$ for $2 \leq p, q \leq m$. For a fixed $m \times m$ proper Gram matrix $G$,

$$Q^d_m(G; X) := N_{m-2}[G]e_1e_1^T + \sum_{u_1 = \alpha} N_{m-1}[G; u](e_1e_u + e_u e_1^T + e_1 e_u^T) + \sum_{u_1 = v_1 = \alpha} (N_m[G; u, v, \alpha] + N_m[G; u, v, -\alpha]) e_u e_v^T \geq 0.$$

For $k \geq 1$,

$$Q^d_m(G; X) := \sum_{u_1 = \alpha} N_{m-1}[G; u]Q_k^d(m)(G; u, 1) e_u e_u^T + \sum_{u_1 = v_1 = \alpha} (N_m[G; u, v, \alpha]Q_k^d(m)(G; u, v, \alpha) + N_m[G; u, v, -\alpha]Q_k^d(m)(G; u, v, -\alpha)) e_u e_v^T \geq 0.$$

**Proof.** We first prove the statement for $k = 0$. By Corollary 2.14(a), for any $G' = \Lambda G A$ where $\Lambda$ is a diagonal matrix with diagonal entries $\pm 1$,

$$Q^d_m(G'; X) = N_{m-2}(\Lambda G A)e_1e_1^T + \sum_{u \in A^m} N_{m-1}(\Lambda G A; \Lambda e_u)(e_1e_{\Lambda e_u}^T + e_{\Lambda e_u} e_1^T + e_{\Lambda e_u} e_{\Lambda e_u}^T) + \sum_{u, v \in A^m} (N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, \alpha) + N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, -\alpha)) (e_{\Lambda e_u} e_{\Lambda e_v}^T) \geq 0. \tag{3.1}$$

Let $S$ be the linear transformation defined by $S(e_1) = e_1$, $S(e_u) = e_u$ for $u_1 = \alpha$, and $S(e_u) = e_{-u}$ for $u_1 = -\alpha$. By conjugating $S$ on (3.1), we have

$$N_{m-2}(\Lambda G A)e_1e_1^T + \sum_{u \in A^m} N_{m-1}(\Lambda G A; \Lambda u)(e_1(S e_u)^T + (S e_u) e_1^T + (S e_u) (S e_u)^T) + \sum_{u, v \in A^m} (N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, \alpha) + N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, -\alpha)) (S e_u) (S e_v)^T \geq 0,$$

therefore

$$N_{m-2}(\Lambda G A)e_1e_1^T + \sum_{u_1 = \alpha} \sum_{\varepsilon \in \{ \pm 1 \}} N_{m-1}(\Lambda G A; \varepsilon e_u)(e_1 e_u^T + e_u e_1^T + e_u e_u^T) + \sum_{u_1 = v_1 = \alpha} \sum_{\varepsilon, \varepsilon' \in \{ \pm 1 \}} (N_m(\Lambda G A; \varepsilon e_u, \varepsilon' e_v, \alpha) + N_m(\Lambda G A; \varepsilon e_u, \varepsilon' e_v, -\alpha)) e_u e_v^T \geq 0. \tag{3.2}$$

Summing over all $\Lambda$ in (3.2), gives $2Q^d_m(G; X) \geq 0$.

Now we fix $k \geq 1$. By Corollary 2.14(b), for any $G' = \Lambda G A$,

$$Q^d_m(G'; X) = \sum_{u \in A^m} N_{m-1}(\Lambda G A; \Lambda u)Q_k^d(m)(\Lambda G A; \Lambda e_u, 1) e_{\Lambda e_u} e_{\Lambda e_u}^T + \sum_{u, v \in A^m} (N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, \alpha)Q_k^d(m)(\Lambda G A; \Lambda e_u, \Lambda e_v, \alpha) + N_m(\Lambda G A; \Lambda e_u, \Lambda e_v, -\alpha)Q_k^d(m)(\Lambda G A; \Lambda e_u, \Lambda e_v, -\alpha)) e_{\Lambda e_u} e_{\Lambda e_v}^T \geq 0. \tag{3.3}$$
Let $S$ be the linear transformation defined by $S(e_{u_1}) = e_u$ for $u_1 = \alpha$, and $S(e_{u_1}) = (-1)^k e_{-u}$ for $u_1 = -\alpha$. By conjugating $S$ on (3.3) and applying Proposition 3.7, the first term in (3.3) becomes

$$
\sum_{u_1=\alpha} \left( N_{m-1}(\Lambda \alpha G A; A u_1) Q_{k}^{d,m}(\Lambda \alpha G A; A u_1, 1) + (-1)^k N_{m-1}(\Lambda \alpha G A; -A u_1) Q_{k}^{d,m}(\Lambda \alpha G A; -A u_1, -1) \right) e_u e_u^T
$$

and the second term becomes

$$
\sum_{u_1=\alpha} \left( \sum_{\varepsilon,\varepsilon' \in \{\pm 1\}} N_m(\Lambda \alpha G A; \varepsilon A u_1, \varepsilon A v, \varepsilon \varepsilon' \alpha) \right) Q_{k}^{d,m}(G; u, v, \alpha) e_u e_u^T
$$

Therefore, summing over all $\Lambda$ in (3.3) gives $2Q_{k}^{d,m}(G; X) \succeq 0$. \hfill \Box

**Remark 3.9.** After switching reduction, the matrices $Q_{k}^{d,m}(G; X)$ have order $2m-1$ if $k = 0$, and order $2m-1$ if $k \geq 1$. The order is halved in contrast to Corollary 2.14. Furthermore, if $G'$ is switching equivalent to $PGP^T$ for some permutation matrix $P$, then $Q_{k}^{d,m}(G; X)$ and $Q_{k}^{d,m}(G'; X)$ are identical up to relabelling of basis. Therefore, the number of semidefinite constraints of a semidefinite program developed by $(m+2)$-point semidefinite constraints is decreased to $a(m)$ after switching reduction.

### 4 Four-point semidefinite bound for equiangular lines

Yu [13] proved the three-point semidefinite bound, which states that $N_{1/a}(d) \leq (a^2-1)(a^2-2)/2$ for $d \leq D_3(a) = 3a^2 - 16$. The bound was proved by using the three-point semidefinite programming method based on Theorem 2.2. Furthermore, Glazyrin and Yu [13] proved that the constructions attaining this bound must lie in an $(a^2 - 2)$-dimensional subspace. We prove the generalizations of these results, namely, Theorem 1.3 and Theorem 1.4, in this section.

#### 4.1 Proof of Theorem 1.3

We state Theorem 1.3 as follows.

**Theorem 4.1.** Let $a \geq 3$ be an odd integer. Suppose $d \leq \lfloor D_4(a) \rfloor$, where $D_4(a)$ is the maximum root of the equation

$$
g_a(x) := (-7a^{14} - 122a^{12} - 342a^{10} + 2776a^8 + 7049a^6 - 17238a^4 - 22932a^2 - 6048)x^4$$

$$+ 12(4a^{16} + 21a^{14} - 227a^{12} + 46a^{10} + 3338a^8 - 7643a^6 + 2693a^4 + 7140a^2 + 864)x^3$$

$$- 9a^2(11a^{16} - 94a^{14} + 25a^{12} + 3068a^{10} - 13951a^8 + 25882a^6 - 15987a^4 - 9608a^2 + 14800)x^2$$

$$+ 54a^2(a-2)^2(a-1)^2(a+1)^2(a+2)^2(a^2+1)(a^4-a^3-5a^2+3a+10)(a^4+a^3-5a^2-3a+10)x$$

$$- 81a^2(a-2)^4(a-1)^4(a+1)^4(a+2)^4 = 0.$$  

Then

$$N_{1/a}(d) \leq \frac{1}{2}(a^2 - 1)(a^2 - 2).$$
Furthermore, when $a$ tends to infinity,

$$D_4(a) = 3a^2 + \frac{12}{\sqrt{5}}a - \frac{948}{25} + O(a^{-1}).$$

Theorem 3.1 can be proved by using the alternative four-point semidefinite constraints with switching reduction, i.e., Theorem 3.8 with $m = 2$. In the following we fix $\alpha = 1/a$, $G = \begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix}$, $u_1 = (\alpha, \alpha)^\top$ and $u_2 = (\alpha, -\alpha)^\top$. As shown in Example 3.8, the two-point distance distribution of switching classes is $N_0[G] = N(N - 1)$; the three-point distance distribution of switching classes is

$$y_1 := N_1[1; \alpha, \alpha, \alpha], y_2 := N_1[1; \alpha, \alpha, -\alpha];$$

the four-point distance distribution of switching classes is

$$z_1 := N_2[G; u_1, u_1, \alpha], z_2 := N_2[G; u_1, u_1, -\alpha], z_3 := N_2[G; u_2, u_2, -\alpha].$$

By Theorem 3.8,

$$Q^{d,2}_0[G; X] = \begin{pmatrix} N(N-1) & y_1 & y_2 \\ y_1 & y_1 + z_1 + z_2 & 2z_2 \\ y_2 & 2z_2 & y_2 + z_2 + z_3 \end{pmatrix} \succeq 0;$$

for $k \geq 1,

$$Q^{d,2}_k[G; X] = \begin{pmatrix} y_1Q^{d,2}_k(G; u_1, u_1, 1) & z_2Q^{d,2}_k(G; u_1, u_2, \alpha) \\ +z_1Q^{d,2}_k(G; u_1, u_1, \alpha) & +z_2Q^{d,2}_k(G; u_1, u_2, -\alpha) \\ +z_2Q^{d,2}_k(G; u_2, u_1, \alpha) & y_2Q^{d,2}_k(G; u_2, u_2, 1) \\ +z_2Q^{d,2}_k(G; u_2, u_1, -\alpha) & +z_2Q^{d,2}_k(G; u_2, u_2, -\alpha) \\ +z_3Q^{d,2}_k(G; u_2, u_2, -\alpha) \end{pmatrix} \succeq 0.$$

Let $\langle \cdot, \cdot \rangle$ be the Frobenius inner product of matrices defined by $\langle A, B \rangle = \text{tr}(A^\top B)$. By the Schur product theorem, $\langle A, B \rangle \succeq 0$ when both $A$ and $B$ are positive semidefinite. Our goal is to find the dual matrices $\{F_k\}$ such that

$$\sum_k \langle Q^{d,2}_k[G; X], F_k \rangle \succeq 0 \iff N \leq \frac{1}{2}(a^2 - 1)(a^2 - 2).$$

If so, then $N_{1/a}(d)$ has an upper bound $(a^2 - 1)(a^2 - 2)/2$ whenever all the matrices $F_k$ are positive semidefinite.

**Lemma 4.2.** There exists a symmetric $3 \times 3$ matrix $F$ and two real numbers $f_1$, $f_2$ such that

$$\langle Q^{d,2}_0[G; X], F \rangle + \langle Q^{d,2}_3[G; X], \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} \rangle = N(N - 1) \left( \frac{1}{2}(a^2 - 1)(a^2 - 2) - 2 \right) - (y_1 + y_2).$$

**Proof.** Let $F = \begin{pmatrix} F_0 & F_1 & F_2 \\ F_1 & F_3 & F_4 \\ F_2 & F_4 & F_5 \end{pmatrix}$. The matrix $F$ we found has null space

$$\mathbb{R} \begin{pmatrix} 4 \\ (a + 1)^3(a - 2) \\ (a - 1)^3(a + 2) \end{pmatrix}.$$
That is,

\[ 4F_1 + (a + 1)^3(a - 2)F_3 + (a - 1)^3(a + 2)F_4 = 0 \quad \text{(E1)} \]
\[ 4F_2 + (a + 1)^3(a - 2)F_4 + (a - 1)^3(a + 2)F_5 = 0 \quad \text{(E2)} \]

On the other hand, to equate both sides of the equation, the coefficients of the variables in both sides should be the same. Therefore

\[
N(N - 1) : F_0 = \frac{1}{2}(a^2 - 1)(a^2 - 2) - 2 \quad \text{(E3)}
\]
\[
y_1 : (2F_1 + F_3) + Q_3^{d,2}(G; u_1, u_1, 1)f_1 = -1 \quad \text{(E4)}
\]
\[
y_2 : (2F_2 + F_5) + Q_3^{d,2}(G; u_2, u_2, 1)f_2 = -1 \quad \text{(E5)}
\]
\[
z_1 : F_3 + Q_3^{d,2}(G; u_1, u_1, \alpha)f_1 = 0 \quad \text{(E6)}
\]
\[
z_2 : (F_3 + 4F_4 + F_5) + Q_3^{d,2}(G; u_1, u_1, -\alpha)f_1 + Q_3^{d,2}(G; u_2, u_2, \alpha)f_2 = 0 \quad \text{(E7)}
\]
\[
z_3 : F_5 + Q_3^{d,2}(G; u_2, u_2, -\alpha)f_2 = 0 \quad \text{(E8)}
\]

(E1) to (E8) is a system of linear equations. When \((a^4 - 5a^2 + 12) - (a^2 + 7)d \neq 0\), we can solve \(F_0, F_1, F_2, F_3, F_4, F_5, f_1, f_2\) in terms of \(d\) and \(a\). The values of \(f_1\) and \(f_2\) are

\[
f_1 = \frac{a^3(d - 3)\left(3a(a - 2)^2(a + 1)^2 - (a^3 + 9a - 6)d\right)}{3d(a - 2)(a - 1)(a + 1)\left(a^4 - 5a^2 + 12 - (a^2 + 7)d\right)}
\]
\[
f_2 = \frac{-a^3(d - 3)\left(3a(a + 2)^2(a - 1)^2 - (a^3 + 9a + 6)d\right)}{3d(a + 2)(a - 1)(a + 1)\left(a^4 - 5a^2 + 12 - (a^2 + 7)d\right)}
\]

The principal minors of \(F\) are

\[
F_0 = \frac{1}{2}(a^2 - 1)(a^2 - 2) - 2,
\]
\[
F_3 = \frac{(a - 1)^3\left(3(a + 2)^2 - d\right)}{a^3(a + 1)^3(d - 3)} f_1,
\]
\[
F_5 = \frac{-(a + 1)^3\left(3(a - 2)^2 - d\right)}{a^3(a - 1)^3(d - 3)} f_2,
\]
\[
F_0F_3 - F_1^2 = \frac{g_a(d)}{36d^2(a - 2)^2(a + 1)^6\left(a^4 - 5a^2 + 12 - (a^2 + 7)d\right)^2},
\]
\[
F_0F_5 - F_2^2 = \frac{g_a(d)}{36d^2(a + 2)^2(a - 1)^6\left(a^4 - 5a^2 + 12 - (a^2 + 7)d\right)^2},
\]
\[
F_3F_5 - F_4^2 = \frac{4g_a(d)}{9d^2(a - 2)^2(a + 2)^2(a - 1)^6(a + 1)^6\left(a^4 - 5a^2 + 12 - (a^2 + 7)d\right)^2},
\]
\[
\det F = 0.
\]

Note that the polynomial \(g_a(x)\) mentioned in the statement of Theorem 4.1 appears as the numerator of the \(2 \times 2\) principal minors of \(F\).
**Proof of Theorem 4.1.** By Lemma 4.2 if \( f_1, f_2 \) and all the principal minors of \( F \) are nonnegative, then
\[
0 \leq \left\langle Q^d_0[G;X], F \right\rangle + \left\langle Q^d_3[G;X], \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} \right\rangle = N(N-1) \left( \frac{1}{2}(a^2 - 1)(a^2 - 2) - N \right)
\]

\[\implies N \leq \frac{1}{2}(a^2 - 1)(a^2 - 2).\]

For \( a = 3 \), \( D_4(3) \approx 14.42 \) and \( |D_4(3)| = 14 \); for \( a \geq 5 \), one can check that the leading coefficient of \( g_a(x) \) is negative, and the equation \( g_a(x) = 0 \) has four real roots in the disjoint intervals
\[
\left[0, \frac{3}{2a^2}\right], \left[\frac{6}{7}a^2 - 8, \frac{6}{7}a^2\right], \\
\left[3a^2 - \frac{12}{\sqrt{5}} - \frac{948}{25}, \frac{30\sqrt{5}}{a} - 3a^2 - \frac{12}{\sqrt{5}}\right], \\
\left[3a^2 + \frac{12}{\sqrt{5}} - \frac{948}{25}, \frac{32\sqrt{5}}{a} + 3a^2 + \frac{12}{\sqrt{5}}\right],
\]
which proves the asymptotic argument of \( D_4(a) \). In addition, we have
\[
3a^2 + \frac{12}{\sqrt{5}} - \frac{948}{25} - \frac{32\sqrt{5}}{a} \leq 1 \leq |D_4(a)| \leq 3a^2 + \frac{12}{\sqrt{5}} - \frac{948}{25} + \frac{2\sqrt{5}}{a},
\]

In either case, when taking \( d = |D_4(a)| \), one can check that \( f_1, f_2 \) and all the principal minors of \( F \) except \( \det F \) are positive. Therefore
\[
N_{1/a}(d) \leq \frac{1}{2}(a^2 - 1)(a^2 - 2)
\]
whenever \( d \leq |D_4(a)| \).

\[\square\]

**Remark 4.3.** Theorem 4.1 explained the numerical results by de Laat et al. [13] partially. By the four-point semidefinite programming method, which is denoted by \( \Delta_4(G)^* \) by [13],
\[
N_{1/5}(65) \leq 276, \ N_{1/7}(145) \leq 1128, \ N_{1/9}(251) \leq 3160, \ N_{1/11}(381) \leq 7140,
\]
while the largest applicable dimensions we found are
\[
|D_4(5)| = 64, \ |D_4(7)| = 144, \ |D_4(9)| = 250, \ |D_4(11)| = 380.
\]

**Remark 4.4.** Lemma 4.2 can be understood as the duality of semidefinite programming. The found dual matrix \( F \) paired with \( Q^d_0[G;X] \) is a matrix with the null space
\[
\mathbb{R} \begin{pmatrix} (a + 1)^3(a - 2)/4 \\ (a - 1)^3(a + 2)/4 \end{pmatrix}.
\]

This is consistent with the fact that, all the known constructions attaining the bound in Theorem 4.1 satisfy
\[
Q^d_0[G;X] = N(N-1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} (a + 1)^3(a - 2)/4 & (a - 1)^3(a + 2)/4 \\ (a - 1)^3(a + 2)/4 & (a + 1)^3(a - 2)/4 \end{pmatrix},
\]
which is a rank-1 matrix. On the other hand, the found dual matrix paired with \( Q^d_3[G;X] \) is a diagonal matrix. The off-diagonal entries are irrelevant, since the off-diagonal entry in \( Q^d_3[G;X] \) is
\[
z_2 \left( Q^d_3(G;u, u_2, \alpha) + Q^d_3(G;u, u_2, -\alpha) \right),
\]
which must be zero.
4.2 Proof of Theorem 1.4

Glazyrin and Yu [15] proved that the constructions attaining the three-point semidefinite bound must lie in an \((a^2 - 2)\)-dimensional subspace. As a generalization, Theorem 1.4 states that the constructions attaining the four-point semidefinite bound must lie in an \((a^2 - 2)\)-dimensional subspace as well. Therefore Theorem 1.4 gives restrictions for the constructions of equiangular lines with cardinality \((a^2 - 1)(a^2 - 2)/2\) and inner product \(1/a\) for dimensions \(d \in (D_3(a), D_4(a))\).

If a spherical projection \(X\) is given by choosing an unit vector \(b\) along one line, and then choosing unit vectors with positive inner products with \(b\) along the other lines, then \(X \setminus \{b\}\) is called the derived code of the set of equiangular lines with respect to \(b\).

The proof by Glazyrin and Yu [15] analyzes the structure of the derived codes, of which the two-point distance distributions are known from the linear programming method. However, our proof of Theorem 1.3 cannot determine the distance distributions of derived codes directly. Instead, we consider the distance distribution with two fixed points, and show that the distribution can be determined if the matrix \(Q^d,2_0[G; X]\) in the semidefinite constraint has rank 1, which is the case when \(d < D_4(a)\).

**Lemma 4.5.** Let \(a \geq 3\) be an odd integer and \(d < D_4(a)\). Suppose \(X\) is a spherical projection of a set of equiangular lines in \(\mathbb{R}^d\) with cardinality \((a^2 - 1)(a^2 - 2)/2\) and inner product \(1/a\). Then the matrix \(Q^d,2_0[G; X]\) is of rank 1.

**Proof.** Without the loss of generality, we may assume that \(d = \lfloor D_4(a) \rfloor\). As in the proof of Theorem 4.1,

\[
0 \leq \left\langle Q^d,2_0[G; X], F \right\rangle + \left\langle Q^d,2_3[G; X], \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} \right\rangle = N(N - 1) \left(\frac{1}{2}(a^2 - 1)(a^2 - 2) - N\right) = 0,
\]

therefore both \(\left\langle Q^d,2_0[G; X], F \right\rangle\) and \(\left\langle Q^d,2_3[G; X], \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} \right\rangle\) are zero. Recall that for two positive semidefinite \(n \times n\) matrices \(A, B\) with \(\langle A, B \rangle = 0\), we have the inequality \(\text{rank}(A) + \text{rank}(B) \leq n\), and all the eigenvectors of \(A\) with positive eigenvalues are in \(\ker B\). For \(d = \lfloor D_4(a) \rfloor\), all the principal minors of \(F\) except \(\det F\) are positive, hence \(F\) is a rank 2 matrix with null space

\[
\mathbb{R} \begin{pmatrix} 1 \\ (a + 1)^3(a - 2)/4 \\ (a - 1)^3(a + 2)/4 \end{pmatrix},
\]

and the rank of the matrix \(Q^d,2_0[G; X]\) is at most 1. Since the matrix is nonzero, the rank is 1 and

\[
Q^d,2_0[G; X] = N(N - 1) \begin{pmatrix} 1 \\ (a + 1)^3(a - 2)/4 \\ (a - 1)^3(a + 2)/4 \end{pmatrix} \begin{pmatrix} 1 & (a + 1)^3(a - 2)/4 & (a - 1)^3(a + 2)/4 \end{pmatrix}.
\]

\(\square\)
Let $b, b' \in X$ be different unit vectors. Consider the distance distribution with two fixed points

$$N_{b,b'} := \# \{ c \in X : G(b, b', c) \sim \begin{pmatrix} 1 & \alpha & \alpha \\ \alpha & 1 & \alpha \\ \alpha & \alpha & 1 \end{pmatrix} \}.$$ 

$$N'_{b,b'} := \# \{ c \in X : G(b, b', c) \sim \begin{pmatrix} 1 & \alpha & \alpha \\ \alpha & 1 & -\alpha \\ \alpha & -\alpha & 1 \end{pmatrix} \}.$$ 

Clearly, we have $N'_{b,b'} = (N - 2) - N_{b,b'}$. Furthermore, the two values can be determined when the matrix $Q_0^{d,2}[G; X]$ is of rank 1.

**Lemma 4.6.** Suppose the matrix

$$Q_0^{d,2}[G; X] = \begin{pmatrix} N(N - 1) & y_1 & y_2 \\ y_1 & y_1 + z_1 + z_2 & 2z_2 \\ y_2 & 2z_2 & y_2 + z_2 + z_3 \end{pmatrix}$$

is of rank 1. Then for any $b, b' \in X$ and $b \neq b'$,

$$N_{b,b'} = \frac{y_1}{N(N - 1)} \text{ and } N'_{b,b'} = \frac{y_2}{N(N - 1)}.$$

**Proof.** Consider the matrix

$$\begin{pmatrix} 1 & N_{b,b'} & N'_{b,b'} \\ N_{b,b'} & (N_{b,b'})^2 & N_{b,b'}N'_{b,b'} \\ N'_{b,b'} & N_{b,b'}N'_{b,b'} & (N'_{b,b'})^2 \end{pmatrix}.$$ 

It is not hard to see that the sum of such matrices over all $(b, b') \in X^2$ with $b \neq b'$ is $Q_0^{d,2}[G; X]$. Since $Q_0^{d,2}[G; X]$ is of rank 1, we have

$$0 = N(N - 1)(y_1 + z_1 + z_2) - y_1^2 = \left( \sum_{b \neq b'} 1 \right) \left( \sum_{b \neq b'} N_{b,b'}^2 \right) - \left( \sum_{b \neq b'} N_{b,b'} \right)^2.$$

Therefore, the values $N_{b,b'}$ for all $b \neq b'$ must be the same and equal $y_1/N(N - 1)$. Similarly, we have $N'_{b,b'} = y_2/N(N - 1)$. 

**Proof of Theorem 1.4** Suppose $a \geq 3$ is an odd integer, $d < D_4(a)$, and $X$ is a spherical projection of a set of equiangular lines in $\mathbb{R}^d$ with cardinality $(a^2 - 1)(a^2 - 2)/2$ and inner product $1/a$. Without the loss of generality, we assume that the spherical projection is chosen such that $X \setminus \{ b \}$ is a derived code for some $b \in X$. Consider a graph $H$ with vertex set $V = X \setminus \{ b \}$, and $(c, c') \in V^2$ forms an edge if and only if $c \cdot c' = \alpha$. We first show that the graph $H$ must be a strongly regular graph with parameters

$$\text{SRG} \left( \frac{a^2(a^2 - 3)}{2}, \frac{(a+1)^3(a-2)}{4}, \frac{(a+1)(a+2)(a^2 - 5)}{8}, \frac{(a+1)^3(a-2)}{8} \right).$$

Indeed, the number of vertices is $v = |V| = N - 1 = a^2(a^2 - 3)/2$. By Lemma 4.3 and Lemma 4.6, we have $N_{c,c'} = (a + 1)^3(a - 2)/4$ and $N'_{c,c'} = (a - 1)^3(a + 2)/4$ for any $c, c' \in X$ and $c \neq c'$. For any $b \in V$, the degree of $b$ in $H$ is

$$\deg_H(b) = \# \{ c \in V : G(b_0, b, c) = \begin{pmatrix} 1 & \alpha & \alpha \\ \alpha & 1 & \alpha \\ \alpha & \alpha & 1 \end{pmatrix} = N_{b_0,b} = \frac{(a+1)^3(a-2)}{4}. $$

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Therefore $H$ is $k$-regular with $k = (a + 1)^2(a - 2)/4$. For nonadjacent vertices $b, b' \in V$, let $\mu$ be the number of the common neighbors of $b$ and $b'$ in $H$. Then there are $(k - \mu)$ neighbors of $b$ which are not neighbors of $b'$, and $(k - \mu)$ neighbors of $b'$ which are not neighbors of $b$. Therefore

$$k = N_{b,b'} = (k - \mu) + (k - \mu) \implies \mu = \frac{k}{2} = \frac{(a + 1)^3(a - 2)}{8}.$$  

By a similar argument, one can show that any two adjacent vertices has $\lambda = (3k - v - 1)/2 = (a + 1)(a + 2)(a^2 - 5)/8$ common neighbors.

Let $M$ be the adjacency matrix of $H$. By the theory of strongly regular graphs, the eigenvalues of $M$ are $k, \frac{k}{a + 1}$ and $-\frac{a^2 + 1}{2}$ with multiplicities $a^2 - 3$ and $v - a^2 + 2$, respectively. Since the derived code $X \setminus \{b_0\}$ is a spherical two-distance set in $S^{d-2}$ with inner product set

$$\begin{cases} \pm \alpha - \alpha^2 \\ 1 - \alpha^2 \end{cases} = \begin{cases} \pm a - 1 \\ a^2 - 1 \end{cases} = \begin{cases} 1 \\ a + 1 \\ -1 \\ a - 1 \end{cases},$$

the Gram matrix of the derived code is

$$I + \frac{1}{a + 1} M - \frac{1}{a - 1} (J - I - M).$$

The eigenvalues of the Gram matrix are $\frac{a^2}{2}$ and 0 with multiplicities $a^2 - 3$ and $v - a^2 + 3$, respectively. Therefore, the unit vectors in the derived code span an $(a^2 - 3)$-dimensional space, and the original set of equiangular lines lie in an $(a^2 - 2)$-dimensional space.

The above proof indicates that the derived code of a construction attaining the four-point semidefinite bound must form a strongly regular graph with parameters

$$\text{SRG} \left( \frac{a^2(a^2 - 3)}{2}, \frac{(a + 1)^3(a - 2)}{4}, \frac{(a + 1)(a + 2)(a^2 - 5)}{8}, \frac{(a + 1)^3(a - 2)}{8} \right).$$

Such strongly regular graphs are known to exist and are unique for $a = 3$ and $a = 5$ (see Seidel \[37\], Goethals and Seidel \[17\]). Therefore, we can determine the uniqueness of some maximum constructions of equiangular lines.

**Corollary 4.7.** The following maximum constructions of equiangular lines are unique up to orthogonal transformations.

(a) 28 equiangular lines in $\mathbb{R}^d$ for $7 \leq d \leq 14$ with $\alpha = 1/3$.

(b) 276 equiangular lines in $\mathbb{R}^d$ for $23 \leq d \leq 64$ with $\alpha = 1/5$.

By Glazyrin and Yu \[15\], Theorem 4, the uniqueness is only known for $7 \leq d \leq 11$ with $\alpha = 1/3$, and $23 \leq d \leq 59$ with $\alpha = 1/5$.

**Remark 4.8.** Delsarte et al. \[14\] proved that $N_{1/3}(d) = 28$ for $7 \leq d \leq 15$. There are at least two maximum constructions in $\mathbb{R}^{15}$. Meanwhile, Cao et al. \[11\] proved that $N_{1/5}(d) = 276$ for $23 \leq d \leq 185$. It is known that there are at least two maximum constructions in $\mathbb{R}^{185}$, so it remains unknown that whether the maximum constructions in $\mathbb{R}^d$ for $65 \leq d \leq 184$ are unique.
Further questions

We have established the four-point semidefinite bound by using the alternative four-point semidefinite constraints with switching reduction, namely, Theorem 3.8 with $m = 2$. The five-point and the six-point semidefinite bounds may be able to be established in a similar way; however, the calculation may be quite complicated.

Question 5.1. Establish the five-point and the six-point semidefinite bounds for equiangular lines.

In the proof of the four-point semidefinite bound, we have also noticed some facts, but we fail to give the insights into them.

Question 5.2.

(a) Give a geometric interpretation of the multi-point Gegenbauer polynomials $Q^{d,m}_{k}(G; u, v, t)$, and prove the switching property (Proposition 3.7) with this interpretation.

(b) Give an explanation for the fact that the four-point semidefinite bound for equiangular lines only depends on the constraints $Q^{d,2}_{k}(G; X)$ for $k = 0$ and $k = 3$, but not any other $k$.

(c) Give a characterization of the set of equiangular lines such that the matrix $Q^{d,m}_{k}(G; X)$ vanishes for some certain $m$, $k$ and proper Gram matrix $G$.

For odd integers $a \geq 3$, the existences of constructions of $(a^2 - 1)(a^2 - 2)/2$ equiangular lines in $\mathbb{R}^{a^2-2}$ with inner product $\alpha = 1/a$ are of much importance. By Theorem 1.3 if such a construction is found for some $a$, then the values of $N_{1/a}(d)$ are answered for a wide range of $d$. However, such constructions are only known for $a = 3$ and $a = 5$.

Question 5.3. For which odd integers $a \geq 3$ does the maximum cardinality $N_{1/a}(a^2 - 2)$ equal $(a^2 - 1)(a^2 - 2)/2$? If the cardinality $(a^2 - 1)(a^2 - 2)/2$ is not attainable, what is the value of $N_{1/a}(a^2 - 2)$?

The specific family of equiangular lines is also related to tight spherical 5-designs and tight spherical 4-designs introduced by Delsarte et al. [14]. They proved that a tight spherical 5-design in $S^{d-1}$ is a both-end spherical projection of a set of equiangular lines in $\mathbb{R}^{d}$ with cardinality $d(d+1)/2$ and inner product $\alpha = 1/\sqrt{d+2}$, and a tight spherical 4-design in $S^{d-2}$ is a derived code of a set of equiangular lines in $\mathbb{R}^{d}$ with the same parameters. By Neumann’s Theorem, such constructions of equiangular lines exist only if $d \leq 3$ or $1/\alpha$ is an odd integer.

Question 5.3 is equivalent to classify tight spherical 5-designs and tight spherical 4-designs. The only known constructions for tight spherical 5-designs are in $S^{3}$, $S^{6}$ and $S^{22}$; the only known constructions for tight spherical 4-designs are in $S^{1}$, $S^{5}$ and $S^{21}$. Furthermore, Bannai et al. [6], Nebe and Venkov [33] proved that the tight spherical 5-designs in $S^{a^2-3}$ as well as tight spherical 4-designs in $S^{a^2-4}$ do not exist for $a = 7, 9, 13, 21, 25, 45, 57, 61, 69, 85, 93, \ldots$. Our numerical experiments suggest that the multi-point semidefinite programming method for $m \leq 4$ may not be able to show the nonexistence for any other $a$.

On the other hand, for $a = 5$ Cao et al. [11] proved that $N_{1/5}(d) = 276$ for $23 \leq d \leq 185$. Corollary 1.7 indicated that the constructions of 276 equiangular lines in $\mathbb{R}^{d}$ for $23 \leq d \leq 64$ are unique. However, the number of different maximum constructions for $d > 64$ is not known well.

Question 5.4. What is the number of different constructions of 276 equiangular lines in $\mathbb{R}^{d}$ for $65 \leq d \leq 185$ with $\alpha = 1/5$?

As indicated in Remark 2.4, the alternative semidefinite constraints $Q^{d}(X)$ is simpler than the original one developed by Bachoc and Vallentin [3] when the concerned object $X$ is a spherical
s-distance set. The alternative constraints may be also useful when concerning objects other than sets of equiangular lines.

**Question 5.5.** Derive new results of the maximum cardinality of spherical s-distance sets or new non-existences of strongly regular graphs using the alternative semidefinite constraints.

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**A Research review on equiangular lines**

**A.1 Previous results on N(d)**

Table 4 records the current known lower and upper bounds for $N(d)$ as well as their references.

| $d$  | $N(d)$ | construction | upper bound |
|------|--------|--------------|-------------|
| 2    | 3      | Haantjes [23] | Haantjes [23] |
| 3-4  | 6      | van Lint and Seidel [42] | van Lint and Seidel [42] |
| 5    | 10     | van Lint and Seidel [42] | van Lint and Seidel [42] |
| 6    | 16     | van Lint and Seidel [42] | Lemmens and Seidel [27] |
| 7-13 | 28     | van Lint and Seidel [42] | Greaves et al. [21] |
| 14   | 28     | van Lint and Seidel [42] | Lemmens and Seidel [27] |
| 15   | 36     | Bussemaker and Seidel [16] | Greaves et al. [21] |
| 16   | 40     | Higman [24] | Greaves et al. [21] |
| 17   | 48     | Lemmens and Seidel [27], Greaves et al. [19] | Greaves et al. [22] |
| 18   | 57-60  | Greaves et al. [22] | Greaves [20] |
| 19   | 72-74  | Taylor [41] | Greaves et al. [21] |
| 20   | 90-94  | Taylor [41] | Greaves et al. [21] |
| 21   | 126    | Taylor [41] | Lemmens and Seidel [27] |
| 22   | 176    | Goethals and Seidel [16], Taylor [41] | Lemmens and Seidel [27] |
| 23   | 276    | Goethals and Seidel [16], Taylor [41] | Lemmens and Seidel [27] |
| 24-41| 276    | Goethals and Seidel [16], Taylor [41] | Barg and Yu [8], Yu [43] |
| 42   | 276-288| Goethals and Seidel [16], Taylor [41] | Barg and Yu [8], Yu [43] |
| 43   | 344    | Taylor [41] | Barg and Yu [8], Yu [43] |

Table 4: Lower and upper bounds for $N(d)$

Below is a brief review for the bounds for $N(d)$ in small dimensions:

- Haantjes [23] proved that $N(3) = N(4) = 6$.
- van Lint and Seidel [42] determined $N(5)$ and $N(6)$ and constructed 28 equiangular lines in $\mathbb{R}^7$. They also proved that $N_{1/a}(d) \leq d(a^2 - 1)/(a^2 - d)$ for $d < a^2$, which is known as the relative bound.
- Gerzon [27] proved that $N(d) \leq d(d+1)/2$. This bound is known as the absolute bound. The equality occurs only if $d = 1, 2, 3$, or $a^2 - 2$ for some odd integer $a$. Neumann [27] proved that
a set $X$ of equiangular lines in $\mathbb{R}^d$ with $|X| > 2d$ must have inner product $\alpha$ being reciprocal of an odd integer.

- Lemmens and Seidel [27] collected the maximum known constructions of equiangular lines in dimensions 15-17, 19-23 and 43. Most of the constructions can be found in Taylor’s thesis [41]. An explicit construction of 48 equiangular lines in $\mathbb{R}^{17}$ can be found in Greaves et al. [19]. Lemmens and Seidel also determined $N(d)$ for $d = 7$-$13$, 15 and 21-$23$ by Neumann’s theorem, the relative bound and some analysis on pillars.

- Barg and Yu [8] showed numerically that $N_{1/5}(d) = 276$ for $23 \leq d \leq 60$ by the semidefinite programming method. The results can determine that $N(d) = 276$ for $24 \leq d \leq 41$, $N(42) \leq 288$ and $N(43) = 344$. A rigorous proof of the numerical results is given by Yu [43].

- The maximum known construction in $\mathbb{R}^{18}$ was the same as $\mathbb{R}^{17}$ until Szöllösi [40] found a construction of equiangular lines with cardinality 54. Later, Lin and Yu [30] and Greaves et al. [22] found constructions with cardinalities 56 and 57, respectively.

- For $d = 14, 16$-$20$, all the best possible constructions have inner products $\alpha = 1/5$ (Lemmens and Seidel [27]). The following are the improvements of the upper bounds:

1. $N(14)$: $30$ (relative bound) $\rightarrow 29$ (Greaves et al. [19]) $\rightarrow 28$ (Greaves et al. [21]).
2. $N(16)$: $42$ (relative bound) $\rightarrow 41$ (Greaves et al. [19]) $\rightarrow 40$ (Greaves et al. [21]).
3. $N(17)$: $51$ (relative bound) $\rightarrow 50$ (Sustik et al. [39]) $\rightarrow 49$ (Greaves and Yatsyna [18]) $\rightarrow 48$ (Greaves et al. [22]).
4. $N(18)$: $61$ (relative bound) $\rightarrow 60$ (Greaves [20]).
5. $N(19)$: $76$ (relative bound) $\rightarrow 75$ (Azarija and Marc [1]) $\rightarrow 74$ (Greaves et al. [21]).
6. $N(20)$: $96$ (relative bound) $\rightarrow 95$ (Azarija and Marc [2]) $\rightarrow 94$ (Greaves et al. [21]).

For the asymptotic lower bound, Taylor [41] proved that $N(q^2 - q + 1) \geq q^3 + 1$ for odd prime powers $q$. This construction indicates that $N(d) = \Omega(d^{3/2})$. de Caen [12] proved that $N(d) \geq \frac{2}{9}(d + 1)^2$ for $d = 6 \cdot 4^i - 1$, which implies that

$$\frac{2}{9} \leq \limsup_{d \to \infty} \frac{N(d)}{d^2} \leq \frac{1}{2}.$$ 

Greaves et al. [19] offered another construction, indicating that

$$N(d) \geq \frac{32d^2 + 328d + 296}{1089}.$$ 

### A.2 Previous results on $N_\alpha(d)$

Neumann’s theorem starts the study on $N_{1/a}(d)$ for odd integers $a$. Below is a brief review of the researches on $N_\alpha(d)$.

- For $\alpha = 1/3$, Lemmens and Seidel [27] proved that $N_{1/3}(d) = 28$ for $7 \leq d \leq 15$, and $N_{1/3}(d) = 2(d - 1)$ for $d \geq 15$.

- For $\alpha = 1/5$, Lemmens and Seidel [27] conjectured that $N_{1/5}(d)$ equals 276 for $23 \leq d \leq 185$ and $\lfloor \frac{1}{2}(d - 1) \rfloor$ for $d \geq 185$.

  - Neumaier [34] proved the conjecture for sufficiently large $d$. 

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– Yu [43] proved the conjecture for $23 \leq d \leq 60$.
– Lin and Yu [29] proved that the conjecture is true when the base size $K = 2, 3, 5$, as Lemmens and Seidel claimed.
– Recently, Cao et al. [11] completely proved the conjecture.

• For the asymptotic behavior of $N_\alpha(d)$ as $d \to \infty$,
  – Bukh [9] proved that $N_\alpha(d) = O(d)$ for any $\alpha \in (0, 1)$.
  – Balla et al. [5] proved that $N_\alpha(d) \leq 1.93d$ if $\alpha \neq 1/3$.
  – Jiang and Polyanskii [25] proved that $N_{1/5}(d) = (3/2)d + O(1)$, $N_{1/(1 + 2\sqrt{2})}(d) = (3/2)d + O(1)$, and $N_\alpha(d) \leq 1.49d$ for every $\alpha \neq 1/3, 1/5$ and $1/(1 + 2\sqrt{2})$ and for sufficiently large $d$.
  – Jiang et al. [26] proved that $N_{1/a}(d) = \lfloor \frac{k}{k - 1}(d - 1) \rfloor$ for all sufficiently large $d$, where $k$ is the spectral radius order of $(1 - \alpha)/(2\alpha)$. In particular, $N_{1/a}(d) = \lfloor \frac{k}{k - 1}(d - 1) \rfloor$ for all odd integers $a \geq 3$ and all sufficiently large $d$. If $k = \infty$, then $N_\alpha(d) = d + o(d)$.

• Some new relative bounds.
  – Okuda and Yu [36] proved that
    $$N_{1/a}(d) \leq 2 + (d - 2) \max \left( \frac{(a - 1)^3}{d - (3a^2 - 6a + 2)}, \frac{(a + 1)^3}{(3a^2 + 6a + 2) - d} \right)$$
    for $3a^2 - 6a + 2 < d < 3a^2 + 6a + 2$.
  – Glazyrin and Yu [15] proved that
    $$N_{1/a}(d) \leq \left( \frac{2}{3}a^2 + \frac{4}{7} \right) d + 2$$
    for $a \geq 3$.
  – Balla [4] proved that
    $$N_{1/a}(d) \leq \frac{a^3}{2} \sqrt{d} + \frac{a + 1}{2} d$$
    and
    $$N_{1/a}(d) \leq \max \left( 2a^5 + \frac{2a^4}{a - 1}, (2 + \frac{8}{(a - 1)^2}) (d + 1) \right).$$

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