Complex spherical codes with three inner products

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Abstract

Let X be a finite set in a complex sphere of d dimension. Let $D(X)$ be the set of usual inner products of two distinct vectors in X. A set X is called a complex spherical s-code if the cardinality of $D(X)$ is s and $D(X)$ contains an imaginary number. We would like to classify the largest possible s-codes for given dimension d. In this paper, we consider the problem for the case $s = 3$. Roy and Suda (2014) gave a certain upper bound for the cardinalities of 3-codes. A 3-code X is said to be tight if X attains the bound. We show that there exists no tight 3-code except for dimensions 1, 2. Moreover we make an algorithm to classify the largest 3-codes by considering representations of oriented graphs. By this algorithm, the largest 3-codes are classified for dimensions 1, 2, 3 with a current computer.

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1 Introduction

Let X be a finite set in the d-dimensional complex unit sphere $\Omega(d)$ in $\mathbb{C}^d$. The *angle set* $D(X)$ is defined to be

$$D(X) = \{\boldsymbol{x}^*\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{y} \in X, \boldsymbol{x} \neq \boldsymbol{y}\},$$

where $\boldsymbol{x}^*$ is the transpose conjugate of a column vector $\boldsymbol{x}$. A finite set X is a *complex spherical s-code* if $|D(X)| = s$ and $D(X)$ contains an imaginary number. The value s is called the *degree* of X. For $X, X' \subset \Omega(d)$, we say that X is *isomorphic* to X' if there exists a unitary transformation from X to X'. An s-code $X \subset \Omega(d)$ is *largest* if X has the largest possible cardinality in all s-codes in $\Omega(d)$. One of major problems on s-codes is to classify the largest s-codes for given s and d.

For the real sphere S^{d-1}, a similar concept to s-codes is well studied [7]. A subset X of S^{d-1} is an *s-distance set* if $|D(X)| = s$. Delsarte, Goethals, and Seidel [7] gave an upper bound

$$|X| \leq \binom{d+s-1}{s} + \binom{d+s-2}{s-1}$$

for an s-distance set X in S^{d-1}. An s-distance set X is *tight* if X attains this bound. A tight s-distance set has the structure of a Q-polynomial association scheme, and becomes a tight spherical $2s$-design [7]. Tight s-distance sets have been classified except for $s = 2$ [1, 2, 4, 16]. The largest 1-distance set in S^{d-1} is the regular simplex. The largest s-distance set in S^1 is the regular $(2s+1)$-gon. The largest 2-distance set in S^{d-1} has been determined for all d except for $d = (2k+1)^2 - 3$ with $k \in \mathbb{N}$ [5, 12, 14, 10]. The largest 3-distance set in S^{d-1} has been determined for $d = 3, 8, 22$ [15, 26]. The largest spherical s-distance set is not known for other (s, d). The classification of largest spherical s-distance sets is still open except for $(s, d) = (1, d), (s, 2), (2, d \leq 7), (2, 23), (3, 3)$.

We have the following upper bound for a 2-code X in $\Omega(d)$ [23, 20].

$$|X| \leq \begin{cases} 2d+1 & \text{if } d \text{ is odd,} \\ 2d & \text{if } d \text{ is even.} \end{cases}$$

A 2-code X is *tight* if X attains this bound. For odd d (*resp.* even d), the existence of a tight 2-code in $\Omega(d)$ is equivalent to that of a doubly regular tournament (*resp.* skew Hadamard matrix) of order d [20]. We have the following upper bound for a 3-code X in $\Omega(d)$ [23].

$$|X| \leq \begin{cases} 4 & \text{if } d = 1, \\ d^2 + 2d & \text{if } d \geq 2. \end{cases}$$

A 3-code X is *tight* if X attains this bound. Roy and Suda [23] proved that a tight 3-code has the structure of a commutative non-symmetric association scheme. In this paper, we show that there exists no tight 3-code except for $d = 1, 2$.

We use complex representations of oriented graphs in order to classify the largest 3-codes in $\Omega(d)$. An oriented graph is a directed graph which has no symmetric pair of directed edges. An oriented graph $G = (V, E)$ is *representable in* $\Omega(d)$ if there exist a mapping φ from V to $\Omega(d)$, an imaginary number α with $\mathrm{Im}(\alpha) > 0$, and a real number β such that for any $u, v \in V$,

$$\varphi(u)^*\varphi(v) = \begin{cases} \alpha & \text{if } (u,v) \in E, \\ \overline{\alpha} & \text{if } (v,u) \in E, \\ \beta & \text{otherwise.} \end{cases}$$

The image of the map φ is called a *complex spherical representation* of G. If two oriented graphs G and G' are not isomorphic, then representations of G and G' are not isomorphic. Let $\boldsymbol{A}$ be the adjacency matrix of G. The Gram matrix $\boldsymbol{H}$ of a complex spherical representation of G can be expressed by

$$\boldsymbol{H} = \boldsymbol{M} + c\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T),$$

for some real number c and some real matrix $\boldsymbol{M}$. Actually $\boldsymbol{M}$ is positive semidefinite. The matrix $\boldsymbol{M}$ can be identified with a real spherical representation of a simple graph G' whose adjacency matrix is $\boldsymbol{A} + \boldsymbol{A}^T$. The dimension of a real spherical representation is studied in [9, 22, 18]. Results related to real representations are helpful to determine the dimension of a complex spherical representation. In this paper, we give an algorithm using only rational arithmetic to classify the largest 3-codes in $\Omega(d)$. By the algorithm, we can classify the largest 3-codes in $\Omega(d)$ for $d = 1, 2, 3$.

This paper is organized as follows. In Section 2, we collect known results of Euclidean representations of a simple graph. In Section 3, we show several results for Hermitian matrices that are used to determine the dimension of complex representation. In Section 4, we consider the dimension of a complex representation of an oriented graph. In Section 5, we give an algorithm to classify the largest 3-codes, and the largest 3-codes in $\Omega(d)$ are classified for $d = 1, 2, 3$ by computer calculation. In Section 6, we show that there exists no tight 3-code except for $d = 1, 2$.

2 Euclidean representations of a simple graph

In this section, we give several results for a real representation of a simple graph. Let V be a finite set of order n, and $E \subset V \times V$. Let G be a graph (V, E). The *adjacency matrix* $\boldsymbol{A}$ of G is the matrix indexed by V, with entries

$$\boldsymbol{A}_{xy} = \begin{cases} 1 & \text{if } (x,y) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Suppose G is simple and G is not a complete graph or a union of isolated vertices. Let $\boldsymbol{A}$ be the adjacency matrix of G, and $\overline{\boldsymbol{A}}$ that of the complement. The matrix $\boldsymbol{M}_c$ is defined to be

$$\boldsymbol{M}_c = c\boldsymbol{A} + \overline{\boldsymbol{A}}$$

for a real number c such that $0 \le c < 1$. A finite set X in $\mathbb{R}^d$ is a *Euclidean representation* or a *real representation* of G if the distance matrix of X is $\boldsymbol{M}_c$ of G for some c. Let $\mathrm{Rep}(G)$ be the smallest integer d such that a Euclidean representation of G is in $\mathbb{R}^d$.

Theorem 1 ([9])**.** *Let G be a simple graph. Let $\boldsymbol{M}_c$ and $\mathrm{Rep}(G)$ be defined as above. Then there exists $\xi \in \mathbb{R}$ such that $0 \le \xi < 1$ and the following hold.*

(1) *$\boldsymbol{M}_\xi$ is the distance matrix in $\mathrm{Rep}(G)$ dimension.*

(2) *For $\xi < c < 1$, $\boldsymbol{M}_c$ is the distance matrix in $n-1$ dimension, and not in $n-2$ dimension.*

(3) *For $0 \le c < \xi$, $\boldsymbol{M}_c$ is not a distance matrix in any dimension.*

A Euclidean representation X of G is a *minimal representation* if the distance matrix of X is $\boldsymbol{M}_\xi$, where ξ is given in Theorem 1. Roy [22] determined $\mathrm{Rep}(G)$ by eigenvalues and eigenspaces of the adjacency matrix of G. Let $\boldsymbol{j}$ be the all-ones column vector.

Theorem 2 ([22, Lemmas 4,5,6, Theorem 7])**.** *Let G be a simple graph with adjacency matrix $\boldsymbol{A}$. Let λ_i be the i-th smallest distinct eigenvalue of $\boldsymbol{A}$, m_i the multiplicity of λ_i, and $\mathcal{E}_i$ the eigenspace corresponding to λ_i. Let $\boldsymbol{P}_i$ be the orthogonal projection matrix onto $\mathcal{E}_i$. Let β_i be the main angle of λ_i, namely, $\beta_i = \sqrt{(\boldsymbol{P}_i \cdot \boldsymbol{j})^T(\boldsymbol{P}_i \cdot \boldsymbol{j})/n}$. Then the following hold:*

(1) *If $\beta_1 = 0$, then $\xi = (\lambda_1+1)/\lambda_1$ and $\mathrm{Rep}(G) = n - m_1 - 1$.*

(2) *If $\beta_1 \neq 0$ and $m_1 > 1$, then $\xi = (\lambda_1+1)/\lambda_1$ and $\mathrm{Rep}(G) = n - m_1$.*

(3) *If $\beta_2 = 0$, $m_1 = 1$, $\lambda_2 < -1$, and $\beta_1^2/(\lambda_2-\lambda_1) = \sum_{i\ge 3}\beta_i^2/(\lambda_i-\lambda_2)$, then $\xi = (\lambda_2+1)/\lambda_2$ and $\mathrm{Rep}(G) = n - m_2 - 2$.*

(4) *If $\beta_2 = 0$, $m_1 = 1$, $\lambda_2 < -1$, and $\beta_1^2/(\lambda_2-\lambda_1) > \sum_{i\ge 3}\beta_i^2/(\lambda_i-\lambda_2)$, then $\xi = (\lambda_2+1)/\lambda_2$ and $\mathrm{Rep}(G) = n - m_2 - 1$.*

(5) *Otherwise, we have $\xi < (\lambda_1+1)/\lambda_1$, $\xi \neq (\lambda_2+1)/\lambda_2$ and $\mathrm{Rep}(G) = n-2$.*

A graph G is of *Type* (i) if G satisfies condition (i) from Theorem 2 for $i \in \{1, \dots, 5\}$. A Euclidean representation X of G is *spherical* if X can be on a sphere.

Theorem 3 ([18])**.** *Let G be a simple graph. Then the following hold.*

(1) *If G is of Type* (1), (2), *or* (4), *then the minimal representation of G is spherical.*

(2) *If G is of Type* (3) *or* (5), *then the minimal representation of G is not spherical.*

(3) *A representation that satisfies condition* (2) *from Theorem* 1 *is spherical.*

A symmetric matrix $\boldsymbol{M}$ is *dissimilarity* if each entry in $\boldsymbol{M}$ is non-negative, and each diagonal entry in $\boldsymbol{M}$ is zero. The smallest integer d such that a dissimilarity matrix $\boldsymbol{M}$ is the distance matrix of some subset X of $\mathbb{R}^d$ is called the *embedding dimension* of $\boldsymbol{M}$. Let $\boldsymbol{P}$ denote the square matrix of order n defined by $\boldsymbol{P} = \boldsymbol{I} - (1/n)\boldsymbol{J}$, where $\boldsymbol{I}$ is the identity matrix and $\boldsymbol{J}$ is the all-ones matrix.

Lemma 1 ([17])**.** *If $\boldsymbol{M}$ is a dissimilarity matrix, then the following equivalent.*

(1) *$\boldsymbol{M}$ is a distance matrix of embedding dimension d.*

(2) *$-\boldsymbol{PMP}$ is a positive semidefinite matrix of rank d.*

Lemma 2 ([17])**.** *If $\boldsymbol{M}$ is a dissimilarity matrix, then the following are equivalent.*

(1) *There uniquely exists $a \in \mathbb{R}$ such that $a > 0$, $-\boldsymbol{M} + a\boldsymbol{J}$ is a positive semidefinite matrix of rank d, $-\boldsymbol{M} + a'\boldsymbol{J}$ is a positive semidefinite matrix of rank $d+1$ for $a' > a$, and $-\boldsymbol{M} + c\boldsymbol{J}$ is not positive semidefinite for $c < a$.*

(2) *$\boldsymbol{M}$ is the distance matrix of a subset of S^{d-1}, where d is the embedding dimension of $\boldsymbol{M}$.*

3 Results on Hermitian matrices

In this section, we give several results for Hermitian matrices that are used later. Let $\boldsymbol{H}$ be a Hermitian matrix of size n. Let λ be an eigenvalue of $\boldsymbol{H}$. Let $\mathcal{E}$ be the eigenspace corresponding to λ. Let $\boldsymbol{P}_\lambda$ be the orthogonal projection matrix onto $\mathcal{E}$. Let $\boldsymbol{j}$ be the all-ones column vector. The *main angle* β of λ is defined to be $\beta = \sqrt{(\boldsymbol{P}_\lambda \cdot \boldsymbol{j})^*(\boldsymbol{P}_\lambda \cdot \boldsymbol{j})/n}$. Note that $\beta = 0$ if and only if $\mathcal{E} \subset \boldsymbol{j}^\perp$. An eigenvalue λ is *main* if $\beta \neq 0$. Let $\boldsymbol{J}$ be the all-ones matrix, and $\boldsymbol{I}$ the identity matrix.

Theorem 4 ([20]). *Let $\boldsymbol{H}$ be a Hermitian matrix, and $\boldsymbol{M} = \boldsymbol{H} + a\boldsymbol{J}$ for a real number a. Let $\tau_1, \dots, \tau_r$ be the distinct main eigenvalues of $\boldsymbol{H}$ such that $\tau_1 < \tau_2 < \cdots < \tau_r$. Let $\mu_1, \dots, \mu_s$ be the distinct main eigenvalues of $\boldsymbol{M}$ such that $\mu_1 < \mu_2 < \cdots < \mu_s$. Let β_i be the main angle of τ_i. Then $r = s$ holds, and*

$$\prod_{i=1}^{r}(\mu_i - x) = \prod_{i=1}^{r}(\tau_i - x)(1 + a\sum_{j=1}^{r}\frac{n\beta_j^2}{\tau_j - x}). \tag{1}$$

Moreover, if $a > 0$, then $\tau_1 < \mu_1 < \tau_2 < \cdots < \tau_r < \mu_r$, and if $a < 0$, then $\mu_1 < \tau_1 < \mu_2 < \cdots < \mu_r < \tau_r$.

Lemma 3. *Let $\boldsymbol{H}$ be a Hermitian matrix of size n. Let $\tau_1, \dots, \tau_r$ be the distinct main eigenvalues of $\boldsymbol{H}$ such that $\tau_1 < \tau_2 < \cdots < \tau_r$. Let β_i be the main angle of τ_i. Let $\boldsymbol{P}$ be the orthogonal projection matrix onto $\boldsymbol{j}^{\perp}$, namely $\boldsymbol{P} = \boldsymbol{I} - (1/n)\boldsymbol{J}$. If $\boldsymbol{H}$ is not positive semidefinite, then the following are equivalent.*

1. (1) *There exists $a \in \mathbb{R}$ such that $a > 0$ and $\boldsymbol{H}+a\boldsymbol{J}$ is positive semidefinite.*
2. (2) *It follows that $\tau_2 > 0$, $\sum_{i=1}^{r}\beta_i^2/\tau_i < 0$, and $\boldsymbol{PHP}$ is positive semidefinite.*

Moreover, if (1) holds, then $a \geq -1/(\sum_{i=1}^{r}n\beta_i^2/\tau_i)$ holds.

Proof. Let λ be an eigenvalue of $\boldsymbol{H}$ that is not main. Let $\boldsymbol{v}$ be a normalized eigenvector corresponding to λ. Note that $\boldsymbol{v}$ is orthogonal to the all-ones vector.

(1) $\Rightarrow$ (2): Since $\boldsymbol{H} + a\boldsymbol{J}$ is positive semidefinite, we have $\lambda = \boldsymbol{v}^*\boldsymbol{H}\boldsymbol{v} = \boldsymbol{v}^*\boldsymbol{P}(\boldsymbol{H}+a\boldsymbol{J})\boldsymbol{P}\boldsymbol{v} \geq 0$. Since $\boldsymbol{H}$ is not positive semidefinite, we have $\tau_1 < 0$. Let $\mu_1, \dots, \mu_r$ be the distinct main eigenvalues of $\boldsymbol{H} + a\boldsymbol{J}$ such that $\mu_1 < \mu_2 < \cdots < \mu_r$. By Theorem 4, we have $\tau_1 < \mu_1 < \tau_2$. Since $\boldsymbol{H} + a\boldsymbol{J}$ is positive semidefinite, we have $0 \leq \mu_1 < \tau_2$. By equation (1) for $x = 0$, it follows that $\sum_{i=1}^{r}n\beta_i^2/\tau_i < 0$ and $a \geq -1/(\sum_{i=1}^{r}n\beta_i^2/\tau_i)$. In particular, $\mu_1 = 0$ if and only if $a = -1/(\sum_{i=1}^{r}n\beta_i^2/\tau_i) > 0$. Since $\boldsymbol{H} + a\boldsymbol{J}$ is positive semidefinite, so is $\boldsymbol{P}(\boldsymbol{H} + a\boldsymbol{J})\boldsymbol{P} = \boldsymbol{PHP}$.

(2) $\Rightarrow$ (1): Since $\boldsymbol{v}$ is orthogonal to the all-ones vector and $\boldsymbol{PHP}$ is positive semidefinite, we have

$$\lambda = \boldsymbol{v}^*\boldsymbol{H}\boldsymbol{v} = \boldsymbol{v}^*\boldsymbol{PHP}\boldsymbol{v} \geq 0. \tag{2}$$

Since $\boldsymbol{H}$ is not positive semidefinite, we have $\tau_1 < 0$. By equation (1) for $x = 0$ and $\tau_2 > 0$, a matrix $\boldsymbol{H} + a\boldsymbol{J}$ is positive semidefinite for $a \geq -1/(\sum_{i=1}^{r}n\beta_i^2/\tau_i) > 0$. $\square$

We can verify the following remarks by the proof of Lemma 3.

Remark 1. If Lemma 3 (1) holds, then

(1) $\mathrm{Rank}(\boldsymbol{H}+a\boldsymbol{J}) = \mathrm{Rank}(\boldsymbol{H}) - 1$ for $a = -1/(\sum_{i=1}^{r} n\beta_i^2/\tau_i)$,

(2) $\mathrm{Rank}(\boldsymbol{H}+a\boldsymbol{J}) = \mathrm{Rank}(\boldsymbol{H})$ for $a > -1/(\sum_{i=1}^{r} n\beta_i^2/\tau_i)$.

Remark 2. If Lemma 3 (2) holds, then the null space of $\boldsymbol{H}$ is contained in $\boldsymbol{j}^{\perp}$.

Remark 3. If Lemma 3 (2) holds, then $\mathrm{Rank}(\boldsymbol{H}+a\boldsymbol{J}) = \mathrm{Rank}(\boldsymbol{PHP})$ for $a = -1/(\sum_{i=1}^{r} n\beta_i^2/\tau_i)$.

Theorem 5. *Let $\boldsymbol{H}$ be a Hermitian matrix. Let $\boldsymbol{M}$ and $\boldsymbol{A}$ be the real matrices such that $\boldsymbol{H} = \boldsymbol{M} + \sqrt{-1}\boldsymbol{A}$. Let $\mathcal{E}_0$ be the null space of $\sqrt{-1}\boldsymbol{A}$. Let $\mathcal{E}_0'$ be the null space of $\boldsymbol{M}$. If $\boldsymbol{H}$ is positive semidefinite, then $\mathcal{E}_0' \subseteq \mathcal{E}_0$ holds.*

Proof. Since $\boldsymbol{M}$ is a real symmetric matrix, we can take a basis of $\mathcal{E}_0'$ consisting of real vectors. For a real vector $\boldsymbol{v} \in \mathcal{E}_0'$, we have

$$\boldsymbol{v}^*\boldsymbol{H}\boldsymbol{v} = \boldsymbol{v}^*\boldsymbol{M}\boldsymbol{v} + \sqrt{-1}\boldsymbol{v}^*\boldsymbol{A}\boldsymbol{v} = 0$$

because $\boldsymbol{A}$ is skew-symmetric. Since $\boldsymbol{H}$ is a positive semidefinite, $\boldsymbol{v}^*\boldsymbol{H}\boldsymbol{v} = 0$ if and only if $\boldsymbol{H}\boldsymbol{v} = \boldsymbol{o}$. It thus follows that

$$\boldsymbol{o} = \boldsymbol{H}\boldsymbol{v} = \boldsymbol{M}\boldsymbol{v} + \sqrt{-1}\boldsymbol{A}\boldsymbol{v} = \sqrt{-1}\boldsymbol{A}\boldsymbol{v}.$$

Therefore $\mathcal{E}_0' \subseteq \mathcal{E}_0$ holds. □

Theorem 6. *Let $\boldsymbol{H}$ be a Hermitian matrix. Let $\boldsymbol{M}$ and $\boldsymbol{A}$ be the real matrices such that $\boldsymbol{H} = \boldsymbol{M} + \sqrt{-1}\boldsymbol{A}$. If $\boldsymbol{H}$ is positive semidefinite, then* $2\mathrm{Rank}(\boldsymbol{H}) \geq \mathrm{Rank}(\boldsymbol{M})$.

Proof. By Theorem 5, we have $\mathcal{E}_0' \subseteq \mathcal{E}_0$. Let $\mathcal{E}_+$ (*resp.* $\mathcal{E}_-$) be the direct sum of eigenspaces corresponding to the positive (*resp.* negative) eigenvalues of $\sqrt{-1}\boldsymbol{A}$. It is easily proved that $\dim \mathcal{E}_+ = \dim \mathcal{E}_-$. For a non-zero vector $\boldsymbol{v} \in \mathcal{E}_+ \oplus ((\mathcal{E}_0')^{\perp} \cap \mathcal{E}_0)$, we have $\boldsymbol{v}^*\boldsymbol{H}\boldsymbol{v} > 0$ because $\boldsymbol{M}$ is positive semidefinite. Therefore,

$$\begin{aligned}
\mathrm{Rank}(\boldsymbol{H}) &\geq \dim(\mathcal{E}_+ \oplus ((\mathcal{E}_0')^{\perp} \cap \mathcal{E}_0)) \\
&= \dim(\mathcal{E}_+) + \dim((\mathcal{E}_0')^{\perp} \cap \mathcal{E}_0) \\
&= \dim(\mathcal{E}_+) + \dim((\mathcal{E}_0')^{\perp}) + \dim(\mathcal{E}_0) - \dim((\mathcal{E}_0')^{\perp} + \mathcal{E}_0) \\
&= \frac{1}{2}\mathrm{Rank}(\boldsymbol{A}) + \mathrm{Rank}(\boldsymbol{M}) + (n - \mathrm{Rank}(\boldsymbol{A})) - n \\
&= \mathrm{Rank}(\boldsymbol{M}) - \frac{1}{2}\mathrm{Rank}(\boldsymbol{A}) \\
&\geq \mathrm{Rank}(\boldsymbol{M}) - \frac{1}{2}\mathrm{Rank}(\boldsymbol{M}) \\
&= \frac{1}{2}\mathrm{Rank}(\boldsymbol{M}),
\end{aligned}$$

where n is the size of $\boldsymbol{H}$. Thus the theorem follows. □

Theorem 7. *Let $\boldsymbol{H}$ be a Hermitian matrix. Let $\boldsymbol{M}$ and $\boldsymbol{A}$ be the real matrices such that $\boldsymbol{H} = \boldsymbol{M} + \sqrt{-1}\boldsymbol{A}$. Let $\mathcal{E}_0$ be the null space of $\sqrt{-1}\boldsymbol{A}$. Let $\mathcal{E}_0'$ be the null space of $\boldsymbol{M}$. Suppose $\boldsymbol{M}$ is positive semidefinite, and $\mathcal{E}_0' \subseteq \mathcal{E}_0$ holds. Then there uniquely exists $\eta > 0$ such that the following hold:*

(1) $\boldsymbol{M} + \eta\sqrt{-1}\boldsymbol{A}$ *is positive semidefinite, and its rank is smaller than* $\mathrm{Rank}(\boldsymbol{M})$*.*

(2) $\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A}$ *is positive semidefinite for $0 \leq c < \eta$, and its rank is equal to* $\mathrm{Rank}(\boldsymbol{M})$*.*

(3) $\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A}$ *is not positive semidefinite for $\eta < c$.*

Proof. Let $\Phi(c)$ be the function defined by

$$\Phi(c) := \min_{\boldsymbol{v} \in (\mathcal{E}_0')^{\perp}, \boldsymbol{v}^*\boldsymbol{v}=1} \boldsymbol{v}^*(\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A})\boldsymbol{v}.$$

Note that $\Phi(c) \geq 0$ if and only if $\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A}$ is positive semidefinite, and $\mathrm{Rank}(\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A}) \leq \mathrm{Rank}(\boldsymbol{M})$. In particular, $\Phi(c) = 0$ if and only if $\mathrm{Rank}(\boldsymbol{M} + c\sqrt{-1}\boldsymbol{A}) < \mathrm{Rank}(\boldsymbol{M})$. Since $\Phi(c)$ is the minimum value of the collection of linear functions in c, the function $\Phi(c)$ is concave. Since $\boldsymbol{M}$ is positive semidefinite, we have $\Phi(0) > 0$. There exists $\boldsymbol{v} \in (\mathcal{E}_0')^{\perp}$ such that $\boldsymbol{v}^*(\sqrt{-1}\boldsymbol{A})\boldsymbol{v} < 0$. It therefore follows that $\lim_{c\to\infty} \Phi(c) = -\infty$. By the intermediate value theorem, this theorem follows. $\square$

4 Representations of an oriented graph

Let X be a complex spherical 3-code with angle set $D(X) = \{\alpha, \overline{\alpha}, \beta\}$, where α is an imaginary number with $\mathrm{Im}(\alpha) > 0$, and $\beta \in \mathbb{R}$. Let $E = \{(\boldsymbol{x}, \boldsymbol{y}) \in X \times X \mid \boldsymbol{x}^*\boldsymbol{y} = \alpha\}$, and $E' = \{(\boldsymbol{x}, \boldsymbol{y}) \mid (\boldsymbol{x}, \boldsymbol{y}) \in E \text{ or } (\boldsymbol{y}, \boldsymbol{x}) \in E\}$. Let G be the oriented graph (X, E) with adjacency matrix $\boldsymbol{A}$. Let G' be the simple graph (X, E') with adjacency matrix $\boldsymbol{B}$. Let $\overline{\boldsymbol{B}}$ be the adjacency matrix of the complement of G'. The Gram matrix $\boldsymbol{H}$ of a complex spherical representation of G can be expressed by

$$\boldsymbol{H} = \boldsymbol{M} + c\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T)$$

for a real number c and a real matrix $\boldsymbol{M}$. Let ϕ be a map from $\Omega(d)$ to S^{2d-1} defined by

$$\phi(u_1 + v_1\sqrt{-1}, \ldots, u_d + v_d\sqrt{-1}) = (u_1, v_1, \ldots, u_d, v_d).$$

Note that $\phi(\boldsymbol{x})^T\phi(\boldsymbol{y}) = \mathrm{Re}(\boldsymbol{x}^*\boldsymbol{y})$ for $\boldsymbol{x}, \boldsymbol{y} \in \Omega(d)$. The matrix $\boldsymbol{M}$ is the Gram matrix of $\phi(X) = \{\phi(\boldsymbol{x}) \mid \boldsymbol{x} \in X\}$. The representation $\phi(X)$ of G' is spherical. By Lemma 2, $\boldsymbol{M}$ can be expressed by

$$\boldsymbol{M} = -(b\boldsymbol{B} + \overline{\boldsymbol{B}}) + a\boldsymbol{J}$$

for $a > 0$ and $b \geq 0$. Note that $b\boldsymbol{B} + \overline{\boldsymbol{B}}$ is the distance matrix of $\phi(X)$ after rescaling the two distances to 1 and b. Since $\phi(X)$ is spherical, $\phi(X)$ is the minimal representation of G' of Type (1), (2) or (4), or a non-minimal representation by Theorem 3.

By Theorem 5, the null space $\mathcal{E}_0'$ of $\boldsymbol{M}$ must be contained in the null space $\mathcal{E}_0$ of $\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T)$. When we consider a minimal-dimensional representation of a given oriented graph G, the minimal representation of G' rarely satisfies $\mathcal{E}_0' \subseteq \mathcal{E}_0$. We give simple examples:

$$G_1 : \boldsymbol{A}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad G_2 : \boldsymbol{A}_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Then both G_1' and G_2' are the cycle C_4. Indeed C_4 is of Type (1), and its minimal representation is the vertex set of the square in $\mathbb{R}^2$. The Gram matrix of the square can be expressed by

$$\boldsymbol{M}_1 = -(\frac{1}{2}\boldsymbol{B} + \overline{\boldsymbol{B}}) + \frac{1}{2}\boldsymbol{J} = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$

The null space of $\boldsymbol{M}_1$ is $\mathrm{Span}\{(1,0,1,0),(0,1,0,1)\}$. This coincides with the null space of $\sqrt{-1}(\boldsymbol{A}_1 - \boldsymbol{A}_1^T)$. Actually we can give a minimal-dimensional representation in $\Omega(1)$ of G_1 as

$$\boldsymbol{H}_1 = -(\frac{1}{2}\boldsymbol{B}+\overline{\boldsymbol{B}})+\frac{1}{2}\boldsymbol{J}+\frac{1}{2}\sqrt{-1}(\boldsymbol{A}_1-\boldsymbol{A}_1^T) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{-1}}{2} & -\frac{1}{2} & -\frac{\sqrt{-1}}{2} \\ -\frac{\sqrt{-1}}{2} & \frac{1}{2} & \frac{\sqrt{-1}}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{\sqrt{-1}}{2} & \frac{1}{2} & \frac{\sqrt{-1}}{2} \\ \frac{\sqrt{-1}}{2} & -\frac{1}{2} & -\frac{\sqrt{-1}}{2} & \frac{1}{2} \end{pmatrix}.$$

On the other hand, the eigenvalues of $\sqrt{-1}(\boldsymbol{A}_2-\boldsymbol{A}_2^T)$ are $\{-\sqrt{2}, -\sqrt{2}, \sqrt{2}, \sqrt{2}\}$, and hence the null space is empty. In this case, $\mathrm{Rank}(\boldsymbol{M}_2)$ must be 4, and we use a non-minimal representation of G':

$$\boldsymbol{M}_2 = -(\boldsymbol{B} + \overline{\boldsymbol{B}}) + \boldsymbol{J} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then we can give a minimal-dimensional representation in $\Omega(2)$ of $\boldsymbol{A}_2$ as

$$\boldsymbol{H}_2 = -(\boldsymbol{B}+\overline{\boldsymbol{B}})+\boldsymbol{J}+\sqrt{\frac{-1}{2}}(\boldsymbol{A}_2-\boldsymbol{A}_2^T) = \begin{pmatrix} 1 & -\sqrt{\frac{-1}{2}} & 0 & -\sqrt{\frac{-1}{2}} \\ \sqrt{\frac{-1}{2}} & 1 & \sqrt{\frac{-1}{2}} & 0 \\ 0 & -\sqrt{\frac{-1}{2}} & 1 & \sqrt{\frac{-1}{2}} \\ \sqrt{\frac{-1}{2}} & 0 & -\sqrt{\frac{-1}{2}} & 1 \end{pmatrix}.$$

The dimension of a non-minimal representation X' of a simple graph G' is $n-1$, where n is the order of G'. If X' is used in order to give a representation X of an oriented graph G, then the dimension d of X is at least $(n-1)/2$ by Theorem 6, namely $n \leq 2d+1$. The union of d triangles that are orthogonal to each other is a spherical 3-code in $\Omega(d)$ and has size $3d$. Therefore it is enough to consider a representation X of G obtained from the minimal representation of G' in order to determine the largest 3-codes.

We consider the minimal-dimensional representation of G obtained from the minimal representation of G'. Throughout this section, we suppose G' has non-zero $\boldsymbol{B}$ and $\overline{\boldsymbol{B}}$, and G' is of Type (1), (2), or (4). Let $\boldsymbol{H}(a,c)$ denote the matrix defined by

$$\boldsymbol{H}(a,c) = -(\xi \boldsymbol{B} + \overline{\boldsymbol{B}}) + a\boldsymbol{J} + c\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T) \tag{3}$$

for real numbers a and c, where ξ is the positive number given in Theorem 1. Note that $\xi \boldsymbol{B} + \overline{\boldsymbol{B}}$ be the distance matrix of the minimal representation of G'. We would like to determine a and c so that $a > 0$, $c > 0$, $\boldsymbol{H}(a,c)$ is positive semidefinite, and the rank of $\boldsymbol{H}(a,c)$ is minimal. Let $\mathcal{E}_0$ be the null space of $\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T)$, and $\mathcal{E}_0'$ be that of $-(\xi \boldsymbol{B} + \overline{\boldsymbol{B}})$.

Remark 4. If G' is of Type (1), (2), or (4), then $\mathcal{E}_0' \subset \boldsymbol{j}^\perp$ holds by Lemma 2 and Remark 2.

Since the diagonal entries in $\boldsymbol{H}(0,c)$ are zero, $\boldsymbol{H}(0,c)$ is not a positive semidefinite. If $\boldsymbol{H}(a,c)$ is positive semidefinite, then $\boldsymbol{H}(0,c)$ satisfies condition (2) from Lemma 3, and hence $\boldsymbol{P}\boldsymbol{H}(0,c)\boldsymbol{P}$ is positive semidefinite. If $\boldsymbol{H}(0,c)$ satisfies condition (2) from Lemma 3, then there uniquely exists a positive number a such that $\mathrm{Rank}(\boldsymbol{H}(a,c))$ is minimal, and $\mathrm{Rank}(\boldsymbol{H}(a,c)) = \mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0,c)\boldsymbol{P})$ by Remarks 1 and 3. Therefore we would like to choose c so that $\boldsymbol{P}\boldsymbol{H}(0,c)\boldsymbol{P}$ is positive semidefinite, and $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0,c)\boldsymbol{P})$ is minimal. The following lemma shows such possible c and the evaluation of $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0,c)\boldsymbol{P})$.

Lemma 4. *Let G be an oriented graph (V,E) with adjacency matrix $\boldsymbol{A}$. Let G' be the simple graph (V,E') with adjacency matrix $\boldsymbol{B}$, where $E' = \{(u,v) \mid (u,v) \in E \text{ or } (v,u) \in E\}$. Let $\overline{\boldsymbol{B}}$ be the adjacency matrix of the complement of G'. Let $\boldsymbol{H}(a,c)$ be the matrix defined by*

$$\boldsymbol{H}(a,c) = -(\xi \boldsymbol{B} + \overline{\boldsymbol{B}}) + a\boldsymbol{J} + c\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T)$$

for real numbers a and c, where ξ is the positive number given in Theorem 1. Let $\mathcal{E}_0$ be the null space of $\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T)$. Let $\mathcal{E}_0'$ be the null space of $-(\xi \boldsymbol{B} + \overline{\boldsymbol{B}})$. If $\mathcal{E}_0' \subseteq \mathcal{E}_0$ holds, then there uniquely exists a positive number η such that

(1) *$\boldsymbol{P}\boldsymbol{H}(0,\eta)\boldsymbol{P}$ is positive semidefinite, and*

$$\mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0,\eta)\boldsymbol{P}) < \mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0,0)\boldsymbol{P}),$$

(2) $\boldsymbol{PH}(0,c)\boldsymbol{P}$ *is positive semidefinite, and*

$$\mathrm{Rank}(\boldsymbol{PH}(0,c)\boldsymbol{P}) = \mathrm{Rank}(\boldsymbol{PH}(0,0)\boldsymbol{P})$$

for $0 < c < \eta$*,*

(3) $\boldsymbol{PH}(0,c)\boldsymbol{P}$ *is not positive semidefinite for* $\eta < c$*.*

Proof. It follows that

$$\boldsymbol{PH}(0,c)\boldsymbol{P} = -\boldsymbol{P}(\xi\boldsymbol{B}+\overline{\boldsymbol{B}})\boldsymbol{P} + c\sqrt{-1}\boldsymbol{P}(\boldsymbol{A}-\boldsymbol{A}^T)\boldsymbol{P}.$$

It is easily shown that the null space of $-\boldsymbol{P}(\xi\boldsymbol{B}+\overline{\boldsymbol{B}})\boldsymbol{P}$ is contained in that of $\sqrt{-1}\boldsymbol{P}(\boldsymbol{A}-\boldsymbol{A}^T)\boldsymbol{P}$. This lemma follows from Theorem 7. $\square$

Next we have to check whether $\boldsymbol{H}(0,c)$ satisfies condition (2) from Lemma 3 for $0 < c \leq \eta$, where η is the positive number given in Lemma 4. If $\boldsymbol{H}(0,c)$ satisfies condition (2) from Lemma 3, we can construct a representation of G by choosing suitable number a.

Theorem 8. *Let G be an oriented graph (V,E) with adjacency matrix $\boldsymbol{A}$. Let G' be the simple graph (V,E') with adjacency matrix $\boldsymbol{B}$, where $E' = \{(u,v) \mid (u,v) \in E \text{ or } (v,u) \in E\}$. Suppose G' is of Type (1), (2), or (4). Let $\overline{\boldsymbol{B}}$ be the adjacency matrix of the complement of G'. Let $\boldsymbol{H}(a,c)$ be the matrix defined by*

$$\boldsymbol{H}(a,c) = -(\xi\boldsymbol{B}+\overline{\boldsymbol{B}}) + a\boldsymbol{J} + c\sqrt{-1}(\boldsymbol{A}-\boldsymbol{A}^T)$$

for real numbers a and c, where ξ is the positive number given in Theorem 1. Let

$$U = \{(a,c) \mid \boldsymbol{H}(a,c) \text{ is positive semidefinite, } a > 0,\ c > 0\},$$

and

$$\mathrm{Rep}(G) = \min\{\mathrm{Rank}(\boldsymbol{H}(a,c)) \mid (a,c) \in U\}.$$

Let $\mathrm{Rep}(G')$ be the dimension of the minimal representation of G'. Let $\mathcal{E}_0$ be the null space of $\sqrt{-1}(\boldsymbol{A}-\boldsymbol{A}^T)$. Let $\mathcal{E}_0'$ be the null space of $-(\xi\boldsymbol{B}+\overline{\boldsymbol{B}})$. Let η be a positive number given in Lemma 4. If $\mathcal{E}_0' \subseteq \mathcal{E}_0$ holds, then the following hold.

(1) *If* $\boldsymbol{H}(0,\eta)$ *satisfies condition* (1) *from Lemma* 3*, then*

$$\mathrm{Rep}(G) = \mathrm{Rank}(\boldsymbol{H}(0,\eta)) - 1 < \mathrm{Rep}(G').$$

(2) *If* $\boldsymbol{H}(0,\eta)$ *does not satisfy condition* (1) *from Lemma* 3*, then*

$$\mathrm{Rep}(G) = \mathrm{Rank}(\boldsymbol{H}(0,0)) - 1 = \mathrm{Rep}(G').$$

Proof. Since the minimal representation of G' is spherical, there uniquely exists $a' \in \mathbb{R}$ such that $\boldsymbol{H}(a', 0)$ is positive semidefinite and $\mathrm{Rep}(G') = \mathrm{Rank}(\boldsymbol{H}(a', 0))$ by Lemma 2. By Remark 3, it follows that $\mathrm{Rank}(\boldsymbol{H}(a', 0)) = \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P})$, and hence

$$\mathrm{Rep}(G') = \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}). \tag{4}$$

Since $\boldsymbol{H}(a, c)$ is positive semidefinite for each $(a, c) \in U$, the matrix $\boldsymbol{PH}(0, c)\boldsymbol{P}$, which is equal to $\boldsymbol{PH}(a, c)\boldsymbol{P}$, is positive semidefinite. Since $\boldsymbol{PH}(0, c)\boldsymbol{P}$ is positive semidefinite and $\mathcal{E}_0' \subseteq \mathcal{E}_0$, it follows that $0 < c \le \eta$,

$$\mathrm{Rank}(\boldsymbol{PH}(0, c)\boldsymbol{P}) = \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}) \tag{5}$$

for $0 < c < \eta$, and

$$\mathrm{Rank}(\boldsymbol{PH}(0, \eta)\boldsymbol{P}) < \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}) \tag{6}$$

for $c = \eta$ by Lemma 4.

If $\boldsymbol{H}(a, c)$ is positive semidefinite, then there uniquely exists $a_c \in \mathbb{R}$ such that $\boldsymbol{H}(a_c, c)$ is positive semidefinite and

$$\mathrm{Rank}(\boldsymbol{PH}(0, c)\boldsymbol{P}) = \mathrm{Rank}(\boldsymbol{H}(a_c, c)) = \mathrm{Rank}(\boldsymbol{H}(0, c)) - 1 \le \mathrm{Rank}(\boldsymbol{H}(a, c)) \tag{7}$$

by Remark 1 and Remark 3.

(1): Since $\boldsymbol{H}(0, \eta)$ satisfies condition (1) from Lemma 3, there exists $a \in \mathbb{R}$ such that $(a, \eta) \in U$. From equations (5), (6) and (7), for each $(a, c) \in U$ with $c \neq \eta$,

$$\begin{aligned} \mathrm{Rank}(\boldsymbol{H}(0, \eta)) - 1 &= \mathrm{Rank}(\boldsymbol{H}(a_\eta, \eta)) = \mathrm{Rank}(\boldsymbol{PH}(0, \eta)\boldsymbol{P}) \\ &< \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}) = \mathrm{Rank}(\boldsymbol{PH}(0, c)\boldsymbol{P}) \\ &= \mathrm{Rank}(\boldsymbol{H}(a_c, c)) \le \mathrm{Rank}(\boldsymbol{H}(a, c)). \end{aligned} \tag{8}$$

For $(a, \eta) \in U$,

$$\mathrm{Rank}(\boldsymbol{H}(0, \eta)) - 1 = \mathrm{Rank}(\boldsymbol{H}(a_\eta, \eta)) \le \mathrm{Rank}(\boldsymbol{H}(a, \eta)) \tag{9}$$

by equation (7). The assertion follows form equations (4), (8), and (9).

(2): Since the minimal representation of G' is spherical, there exists $a' \in \mathbb{R}$ such that $\boldsymbol{H}(a', 0)$ is positive semidefinite. Since $\mathcal{E}_0' \subset \boldsymbol{j}^\perp$ by Remark 4, the null space of $\boldsymbol{H}(a', 0)$ is also $\mathcal{E}_0'$. By Theorem 7, there exists a positive number η' such that $0 < \eta' < \eta$ and $\boldsymbol{H}(a', \eta')$ is positive semidefinite. For each $(a, c) \in U$, it follows from equations (5) and (7) that

$$\begin{aligned} \mathrm{Rank}(\boldsymbol{H}(a_{\eta'}, \eta')) = \mathrm{Rank}(\boldsymbol{PH}(0, \eta')\boldsymbol{P}) &= \mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}) \\ &= \mathrm{Rank}(\boldsymbol{PH}(0, c)\boldsymbol{P}) \le \mathrm{Rank}(\boldsymbol{H}(a, c)). \end{aligned} \tag{10}$$

It follows from Lemma 1 and Remark 1 that

$$\mathrm{Rank}(\boldsymbol{PH}(0, 0)\boldsymbol{P}) = \mathrm{Rank}(\boldsymbol{H}(0, 0)) - 1. \tag{11}$$

The assertion follows from equations (4), (10), and (11). □

5 Algorithm to give the largest 3-codes

In this section, we give an *algorithm* using only rational arithmetic to classify the largest 3-codes in $\Omega(d)$ for given dimension d. First we collect several algorithms used in the *algorithm*. An interval $[a,b]$ is an *isolating interval* for a polynomial f and a real number γ such that $f(\gamma)=0$ if a and b are rational numbers, $a<\gamma<b$, and $[a,b]$ contains no other roots of f. A real algebraic number γ is represented by a pair (f_γ, I), where f_γ is the minimal polynomial of γ over the field of rationals, and I is an isolating interval $[a,b]$ for f and γ. If f is the minimal polynomial of γ, then γ is a simple root and an isolating interval $[a,b]$ satisfies $f(a)f(b)<0$. Since we have an explicit lower bound for the separation of roots of an integral polynomial [24], we easily obtain the isolating interval $[a,b]$.

Lemma 5 ([12])**.** *There is an algorithm (using only rational arithmetic) which takes as input an algebraic number γ and a polynomial f with integer coefficients, and determines the sign of the number $f(\gamma)$.*

Proof. Let g_γ be the minimal polynomial of γ over $\mathbb{Q}$. Since g_γ is irreducible, $f(\gamma)=0$ if and only if g_γ divides f. Suppose g_γ does not divide f. We can find an isolating interval $[a,b]$ for g_γ and γ, such that $[a,b]$ contains no root of f. Then the sign of $f(a)$ is equal to that of $f(\gamma)$. $\square$

Lemma 6. *There is an algorithm (using only rational arithmetic) which takes as input an real algebraic number γ and a symmetric matrix $\boldsymbol{M}(t)$ whose entries are in $\mathbb{Q}[t]$, and determines the number of the positive eigenvalues and the number of the negative eigenvalues of $\boldsymbol{M}(\gamma)$. This decides whether $\boldsymbol{M}(\gamma)$ is positive semidefinite.*

Proof. Let $P(t,x)$ be the polynomial defined by

$$P(t,x)=|\boldsymbol{M}(t)-x\boldsymbol{I}|.$$

Let $P_i(t)$ be the coefficient of x^i in $P(x)=P(t,x)$. By Lemma 5, we can determine the sign of $P_i(\gamma)$. Using Descartes' rule of signs, the number of the positive roots and the number of the negative roots of $P(x)=P(\gamma,x)$ are determined by the list of the signs of $P_i(\gamma)$. $\square$

Let f be an irreducible polynomial over $\mathbb{Q}(\gamma)$ for an algebraic integer γ. Let η be a zero of f. Using Sturm's theorem, η can be represented by (f,I), where I is an isolating interval for f and η. Here the signs in Sturm's sequence can be determined by Lemma 5.

Lemma 7. *There is an algorithm (using only rational arithmetic) which takes as input an algebraic number γ, a real number η that is a root of an irreducible polynomial over $\mathbb{Q}(\gamma)$, and a polynomial f over $\mathbb{Q}(\gamma)$, and determines the sign of the number $f(\eta)$.*

Proof. Suppose that η is represented by (g, I). It follows that $f(\eta) = 0$ if and only if g divides f. By Sturm's theorem, we can find an interval $[a, b]$ such that a and b are rational, $[a, b] \subset I$ and f has no root in I. Then the sign of $f(\eta)$ is the sign of $f(a)$. $\square$

Lemma 8. *There is an algorithm (using only rational arithmetic) which takes as input an real algebraic number γ, a real number η that is a root of an irreducible polynomial over $\mathbb{Q}(\gamma)$ and a symmetric matrix $\boldsymbol{M}(t, c)$ whose entries are in $\mathbb{Q}[t, c]$, and determines the number of the positive eigenvalues and the number of the negative eigenvalues of $\boldsymbol{M}(\gamma, \eta)$. This decides whether $\boldsymbol{M}(\gamma, \eta)$ is positive semidefinite.*

Proof. Let $P(t, c, x)$ be the polynomial defined by

$$P(t, c, x) = |\boldsymbol{M}(t, c) - x\boldsymbol{I}|.$$

Let $P_i(t, c)$ be the coefficient of x^i in $P(x) = P(t, c, x)$. By Lemma 7, we can determine the sign of $P_i(\gamma, \eta)$. Using Descartes' rule of signs, the number of the positive roots and the number of the negative roots of $P(x) = P(\gamma, \eta, x)$ are determined by the list of the signs of $P_i(\gamma, \eta)$. $\square$

Lemma 9. *There is an algorithm (using only rational arithmetic) which takes as input an algebraic number γ and a matrix $\boldsymbol{M}(t)$ whose entries are in $\mathbb{Q}[t]$, and decides whether $\boldsymbol{M}(\gamma)$ is the distance matrix of a spherical set.*

Proof. First we check if $\boldsymbol{M}(\gamma)$ is dissimilarly. Let $P(t, a, x)$ be the polynomial defined by

$$P(t, a, x) = | - \boldsymbol{M}(t) + a\boldsymbol{J} - x\boldsymbol{I}|$$

for indeterminates a and x. Let $P_i(t, a)$ be the coefficient of x^i in $P(x) = P(t, a, x)$. Let $Q_i(t)$ be the coefficient of a^j in $P_i(a) = P_i(t, a)$, where j is the largest exponent that satisfies the coefficient of a^j is not divisible by the minimal polynomial f_γ of γ. If the coefficient of a^j is divisible by f_γ for each j, then we set $Q_i(t) = 0$. By Lemma 5, we can determine the sign of $Q_i(\gamma)$. For sufficient large a, we can determine the sign of $P_i(\gamma, a)$: $P_i(\gamma, a) = 0$ if and only if $Q_i = 0$, $P_i(\gamma, a) > 0$ if and only if $Q_i(\gamma) > 0$, and $P_i(\gamma, a) < 0$ if and only if $Q_i(\gamma) < 0$. Using Descartes' rule of signs, the number m of the negative roots of $P(x) = P(\gamma, a, x)$ for sufficient large a is determined by the list of the signs of $P_i(\gamma, a)$. By Lemma 2, $m = 0$ if and only if $\boldsymbol{M}$ is the distance matrix of a spherical set. $\square$

Lemma 10. *There is an algorithm (using only rational arithmetic) which takes as input an algebraic number γ and a Hermitian matrix $\boldsymbol{H} = \boldsymbol{M} + \sqrt{-1}\boldsymbol{A}$, where $\boldsymbol{M}$ and $\boldsymbol{A}$ are matrices over $\mathbb{Q}(\gamma)$ that satisfy the condition from Theorem 7, and determines a positive real number $\eta = (f, I)$, where η is defined in Theorem 7 and f is over $\mathbb{Q}(\gamma)$.*

Proof. Let $\boldsymbol{H}(c)$ be the matrix $\boldsymbol{M}+c\sqrt{-1}\boldsymbol{A}$. The value η is a unique positive number such that $\boldsymbol{P}\boldsymbol{H}(\eta)\boldsymbol{P}$ is positive semidefinite and $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(\eta)\boldsymbol{P}) < \mathrm{Rank}(\boldsymbol{P}\boldsymbol{H}(0)\boldsymbol{P})$. Let $P(c,x)$ be the polynomial defined by

$$P(c,x) = |\boldsymbol{P}\boldsymbol{H}(c)\boldsymbol{P} - x\boldsymbol{I}|$$

for an indeterminate x. Let $P_i(c)$ be the coefficient of x^i in $P(x) = P(c,x)$. The polynomial $P_i(c)$ is factored into irreducible polynomials over $\mathbb{Q}(\gamma)$ [27]. The rank of $\boldsymbol{P}\boldsymbol{H}(0)\boldsymbol{P}$ is determined by Lemma 6. The value η is determined as the smallest positive zero of $\prod_i P_i(c)$ such that the number of sign differences between consecutive nonzero coefficients $P_i(\eta)$ is smaller than that for $P_i(0)$. $\square$

Lemma 11. *There is an algorithm (using only rational arithmetic) which takes as input an simple graph G, and determines the type of G.*

Proof. Let $\boldsymbol{A}$ be the adjacency matrix of G. Let λ_i be the i-th smallest eigenvalue of $\boldsymbol{A}$, and m_i the multiplicity of λ_i. Indeed there is an algorithm that gives the factorization of an integral polynomial into irreducible polynomials over $\mathbb{Q}$, see [28]. Let $\boldsymbol{M}(t)$ be the matrix defined by $\boldsymbol{M}(t) = -(t+1)\boldsymbol{A} - t\overline{\boldsymbol{A}}$ for an indeterminate t. By Lemma 6, we can determine $\mathrm{Rank}(\boldsymbol{M}(\lambda_i))$ and $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{M}(\lambda_i)\boldsymbol{P})$. By Lemma 1, Remark 1, and Theorems 2, 3, we can determine the type of G as follows. G is Type (1) if and only if $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{M}(\lambda_1)\boldsymbol{P}) = n-m_1-1$ and $\boldsymbol{M}(\lambda_1)$ is the distance matrix of a spherical set. G is Type (2) if and only if $m_1 > 1$, $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{M}(\lambda_1)\boldsymbol{P}) = n - m_1$, and $\boldsymbol{M}(\lambda_1)$ is the distance matrix of a spherical set. G is Type (3) if and only if $m_1 = 1$, $\lambda_2 < -1$, $\boldsymbol{M}(\lambda_2)$ is not the distance matrix of a spherical set, $\boldsymbol{P}\boldsymbol{M}(\lambda_2)\boldsymbol{P}$ is positive semidefinite, and $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{M}(\lambda_2)\boldsymbol{P}) = n-m_2-2$. G is Type (4) if and only if $m_1 = 1$ $\lambda_2 < -1$, $\boldsymbol{M}(\lambda_2)$ is the distance matrix of a spherical set, and $\mathrm{Rank}(\boldsymbol{P}\boldsymbol{M}(\lambda_2)\boldsymbol{P}) = n - m_2 - 1$. If G is not of Type (i) for each $i \in \{1,\dots,4\}$, then G is Type (5). $\square$

Lemma 12. *Let G be a digraph with adjacency matrix $\boldsymbol{A}$. Let G' be either the simple graph with the adjacency matrix $\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{A}^T$ or its complement. Suppose G' is of Type (1), (2), or (4). If the null space of the minimal representation $\xi\boldsymbol{B} + \overline{\boldsymbol{B}}$ is contained in that of $\boldsymbol{A} - \boldsymbol{A}^T$, then there is an algorithm (using only rational arithmetic) which determines* $\mathrm{Rep}(G)$.

Proof. By Lemma 10, we can determine η such that $-\boldsymbol{P}(\xi\boldsymbol{B} + \overline{\boldsymbol{B}})\boldsymbol{P} + \eta\sqrt{-1}\boldsymbol{P}(\boldsymbol{A}-\boldsymbol{A}^T)\boldsymbol{P}$ is a positive semidefinite matrix of rank less than $\mathrm{Rep}(G')$. Note that $\mathrm{Rep}(G')$ is determined by Lemma 11. If there exists a positive number a such that $-(\xi\boldsymbol{B} + \overline{\boldsymbol{B}}) + \eta\sqrt{-1}(\boldsymbol{A} - \boldsymbol{A}^T) + a\boldsymbol{J}$ is positive semidefinite, then $\mathrm{Rep}(G)$ is the rank of $-\boldsymbol{P}(\xi\boldsymbol{B} + \overline{\boldsymbol{B}})\boldsymbol{P} + \eta\sqrt{-1}\boldsymbol{P}(\boldsymbol{A} - \boldsymbol{A}^T)\boldsymbol{P}$, else $\mathrm{Rep}(G) = \mathrm{Rep}(G')$ by Theorem 8. The existence of such a can be checked by a similar manner to Lemma 9. Here the signs of coefficients are checked by Lemma 7. $\square$

We describe the *algorithm* to classify the largest 3-codes in $\Omega(d)$. We first classify simple graphs G' that may give the oriented graphs G whose representations are the largest 3-codes. Let $L_0(\gamma)$ be the all $(2d+2)$-vertex simple graphs G' that represent 2-distance sets in S^{2d-1}, with distances 1 and γ. For $G' \in L_0(\gamma)$, the representation of G' in S^{2d-1} is the minimal representation. The graph in $L_0(\gamma)$ is of Type (1), (2), or (4) by Theorem 3. The distance γ may be less than 1, and $\gamma = (\lambda+1)/\lambda$ holds, where λ is the smallest or second-smallest eigenvalue of G by Theorem 2. First we produce $L_0(\gamma)$ for any possible γ by applying Lemma 11 to all exhaustive simple graphs with $2d+2$ vertices. We have the list of exhaustive simple graphs with at most 10 vertices [13].

Let G' be a simple graph in $L_0(\gamma)$. Let $\boldsymbol{B}$ be the adjacency matrix of G', and $\overline{\boldsymbol{B}}$ the adjacency matrix of the compliment. Let $\boldsymbol{M}(\lambda)$ be the matrix $(\lambda+1)\boldsymbol{B}+\lambda\overline{\boldsymbol{B}}$, where $\lambda = 1/(\gamma-1)$. Let $\mathcal{E}_0'$ be the null space of $\boldsymbol{M}(\lambda)$. Let $K(G')$ be the set of all oriented graphs G such that $\mathcal{E}_0' \subseteq \mathcal{E}_0$, $\boldsymbol{A}+\boldsymbol{A}^T = \boldsymbol{B}$ or $\overline{\boldsymbol{B}}$, and $\mathrm{Rep}(G) \leq d$, where $\boldsymbol{A}$ is the adjacency matrix of G and $\mathcal{E}_0$ be the null space of $\boldsymbol{A}-\boldsymbol{A}^T$. Here $\mathrm{Rep}(G)$ is determined by Lemma 12. Note that $\mathcal{E}_0' \subseteq \mathcal{E}_0$ if and only if the row space of $\boldsymbol{A}-\boldsymbol{A}^T$ is contained in the row space of $\boldsymbol{M}(\lambda)$. Moreover when $\mathrm{Rank}(\boldsymbol{M}(\lambda)) = 2d$ we need $\mathrm{Rank}(\boldsymbol{A}-\boldsymbol{A}^T) = 2d$ in order to have $\mathrm{Rep}(G) = d$ by the proof of Theorem 6. These conditions can reduce a large number of choices of $\boldsymbol{A}$. We can make the list of $\boldsymbol{A}$ and give $\mathrm{Rep}(G)$ for each $\boldsymbol{A}$. If $K(G')$ is empty, then G' is removed from $L_0(\gamma)$. Note that $L_0(\gamma)$ is not empty because the union of d mutually orthogonal equilateral triangles is a 3-code with $3d$ points.

Let $L(n,\gamma)$ be the set of all n-vertex simple graphs G' of Type (1), (2) or (4) such that $K(G')$ is not empty. Now $L(2d+2,\gamma) = L_0(\gamma)$. The list of $L(n+1,\gamma)$ is produced from $L(n,\gamma)$ by the following algorithm based on [12]. Possibilities of augmenting graph $G' \in L(n,\gamma)$ by an $(n+1)$-th vertex are examined. There are 2^n possibilities of a newly added $(n+1)$-th row of $\boldsymbol{B}$. Its entries are in $\{0,1\}$. We may think of these 2^n sequences as leaves of a binary tree of depth n. In depth at least $2d+2$, the search effectively pruned by checking various sub-matrices of size $2d+2$ against the list $L(2d+2,\gamma)$. Let $\tilde{\boldsymbol{B}}$ be a new matrix obtained from $\boldsymbol{B}$ by adding a new column and a new row, and $\tilde{G}'$ the simple graph with the adjacency matrix $\tilde{\boldsymbol{B}}$. We check whether $\tilde{G}'$ already appears in $L(n+1,\gamma)$. If not, then we form the $2d+2$ graphs $\tilde{G}'_i$ for $1 \leq i \leq 2d+2$, where $\tilde{G}'_i$ is the induced subgraph of $\tilde{G}'$ which arises by deleting its vertex i. Since any induced subgraph of $\tilde{G}'$ on $2d+2$ vertices is contained in at least one of the graphs $\tilde{G}'_1, \ldots, \tilde{G}'_{2d+2}$, G', it follows that $\mathrm{Rep}(\tilde{G}') \leq 2d$ if and only if all graphs $\tilde{G}'_1, \ldots, \tilde{G}'_{2d+2}$, G' are appears in $L(n,\gamma)$. If $\tilde{G}'$ is of Type (1), (2), or (4) and $K(\tilde{G}')$ is not empty, then $\tilde{G}'$ is appended to $L(n,\gamma)$.

The smallest number n such that $L(n+1,\gamma)$ is empty for any γ is the size of a largest 3-code. For all G' in $L(n,\gamma)$, the union of the sets $K(G')$ gives the classification of oriented graphs whose complex representations are largest 3-codes.

By the *algorithm* we can classify the largest complex 3-codes in $\Omega(d)$ for $d = 1, 2, 3$. Table 1 shows the number of largest 3-codes.

d	1	2	3
$\lvert X\rvert$	4	8	9
#	1	1	50

Table 1

For $d \geq 4$, a usual computer cannot give the classification. For $d = 1, 2$, the largest complex 3-codes are tight, and they are considered in Section 6. For $d = 3$, one of the largest 3-codes is the union of three equilateral triangles in $\mathbb{C}^1$, which are orthogonal to each other. For the other largest 3-codes X, $\phi(X \cup e^{2\pi\sqrt{-1}/3}X \cup e^{4\pi\sqrt{-1}/3}X)$ is the unique largest 2-distance set in $\mathbb{R}^6$ [7, 25], which is the minimal representation of the Schläfli graph with 27 vertices.

6 Tight complex spherical 3-codes

In this section, we give upper bounds on complex spherical 3-codes and characterize 3-codes achieving the upper bound by using another type of codes, called $\mathcal{S}$-codes. A tight $\mathcal{S}$-code with degree $|\mathcal{S}| - 1$ has the structure of a commutative association scheme. We review the theory of complex spherical designs and codes [23] and commutative association schemes [3].

Let $\mathbb{N}$ denote the set of nonnegative integers. A finite subset $\mathcal{S}$ of $\mathbb{N}^2$ is a *lower set* if the following condition is satisfied: if $(i, j) \in \mathbb{N}^2$ is in $\mathcal{S}$ then so is (k, l) for any $0 \leq k \leq i$ and $0 \leq l \leq j$. A finite set X in $\Omega(d)$ is an *$\mathcal{S}$-code* if there exists a polynomial $F(x) = \sum_{(k,l)\in\mathcal{S}} a_{k,l} x^k \bar{x}^l$ with real coefficients such that $F(\alpha) = 0$ for any $\alpha \in D(X)$ and $F(1) > 0$.

We denote by $\mathrm{Hom}_d(k, l)$ the vector space generated by homogeneous polynomials of degree k in variables $\{z_1, \ldots, z_d\}$ and of degree l in variables $\{\bar{z}_1, \ldots, \bar{z}_d\}$. The unitary group $U(d)$ acts on $\mathrm{Hom}_d(k, l)$, and the irreducible decomposition is

$$\mathrm{Hom}_d(k, l) = \bigoplus_{m=0}^{\min(k,l)} \mathrm{Harm}_d(k - m, l - m),$$

where $\mathrm{Harm}(k, l)$ is the subspace of $\mathrm{Hom}(k, l)$ that is the kernel of the Laplace operator $\Delta = \sum_{i=1}^{d} \partial^2/\partial z_i \partial \overline{z_i}$.

Define an inner product on polynomials f and g on $\Omega(d)$ as follows:

$$\langle f, g\rangle := \int_{\Omega(d)} \overline{f(\boldsymbol{z})} g(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z}.$$

Here $\mathrm{d}\boldsymbol{z}$ is the unique invariant Haar measure on $\Omega(d)$, normalized so that $\int_{\Omega(d)} \mathrm{d}\boldsymbol{z} = 1$. With respect to this inner product, $\mathrm{Harm}_d(k, l)$ is orthogonal to $\mathrm{Harm}_d(k', l')$ whenever $(k, l) \neq (k', l')$. For each $(k, l) \in \mathbb{N}^2$, fix an orthonormal basis $\{e_1, \dots, e_{m^d_{k,l}}\}$ for the space $\mathrm{Harm}_d(k, l)$. For a finite set X in $\Omega(d)$, we define the characteristic matrix $\boldsymbol{H}_{k,l}$ with rows indexed by X and columns indexed by $\{1, 2, \dots, m^d_{k,l}\}$ as

$$(\boldsymbol{H}_{k,l})_{\boldsymbol{x},i} = e_i(\boldsymbol{x})$$

for $\boldsymbol{x} \in X$ and $i \in \{1, 2, \dots, m^d_{k,l}\}$.

For each $(k, l) \in \mathbb{N}^2$, we define a Jacobi polynomial $g^d_{k,l}$ as follows:

$$g^d_{k,l}(x) := \frac{m^d_{k,l}(d-2)!k!l!}{(d+k-2)!(d+l-2)!} \sum_{r=0}^{\min\{k,l\}} (-1)^r \frac{(d+k+l-r-2)!}{r!(k-r)!(l-r)!} x^{k-r}\overline{x}^{l-r},$$

where

$$\begin{aligned} m^d_{k,l} &= \dim(\mathrm{Harm}_d(k, l)) \\ &= \binom{d+k-1}{d-1}\binom{d+l-1}{d-1} - \binom{d+k-2}{d-1}\binom{d+l-2}{d-1}. \end{aligned} \tag{12}$$

The Jacobi polynomials which we used are

$$\begin{aligned} g^d_{0,0}(x) &= 1, \\ g^d_{1,0}(x) &= dx, \\ g^d_{0,1}(x) &= d\overline{x}, \\ g^d_{1,1}(x) &= (d+1)(dx\overline{x} - 1). \end{aligned}$$

Recursively, the Jacobi polynomials satisfy

$$x g^d_{k,l}(x) = a_{k,l} g^d_{k+1,l}(x) + b_{k,l} g^d_{k,l-1}(x), \tag{13}$$

where $a_{k,l} = \frac{k+1}{d+k+l}$, $b_{k,l} = \frac{d+l-2}{d+k+l-2}$ and set $g^d_{k,l}(x) = 0$ unless $(k, l) \in \mathbb{N}^2$.

The essential property of the Jacobi polynomials is the following theorem, known as Koornwinder's addition theorem.

Theorem 9. *Let $\{e_1, \dots, e_{m^d_{k,l}}\}$ be an orthonormal basis for the space* $\mathrm{Harm}_d(k, l)$. *Then for any $\boldsymbol{a}, \boldsymbol{b} \in \Omega(d)$,*

$$\sum_{i=1}^{m^d_{k,l}} \overline{e_i(\boldsymbol{a})} e_i(\boldsymbol{b}) = g^d_{k,l}(\boldsymbol{a}^* \boldsymbol{b}).$$

An upper bound on the size of an $\mathcal{S}$-code is given as follows.

Theorem 10 ([23, Theorem 4.2 (ii)])**.** *For $d \geq 2$, let X be an $\mathcal{S}$-code in $\Omega(d)$. Then $|X| \leq \sum_{(k,l)\in\mathcal{S}} \dim(\mathrm{Harm}(k, l))$ holds.*

An $\mathcal{S}$-code is *tight* if equality holds in Theorem 10. Tight codes are related to complex spherical designs. For a finite lower set $\mathcal{T}$, a finite subset X of $\Omega(d)$ is a *complex spherical $\mathcal{T}$-design* if, for every polynomial $f \in \mathrm{Hom}(k,l)$ such that (k,l) is in $\mathcal{T}$,

$$\frac{1}{|X|}\sum_{\boldsymbol{z}\in X} f(\boldsymbol{z}) = \int_{\Omega(d)} f(\boldsymbol{z})\mathrm{d}\boldsymbol{z}, \tag{14}$$

where $\mathrm{d}\boldsymbol{z}$ is the Haar measure on $\Omega(d)$ normalized by $\int_{\Omega(d)} \mathrm{d}\boldsymbol{z} = 1$. As stated in the following theorem, tight $\mathcal{S}$-codes are complex spherical $\mathcal{S}*\mathcal{S}$-designs, where $\mathcal{S}*\mathcal{S} := \{(k+l', k'+l) \mid (k,l),(k',l') \in \mathcal{S}\}$.

Theorem 11 ([23, Theorem 5.4])**.** *Let X be a finite set in $\Omega(d)$ and let $\mathcal{S}$ be a lower set. Then the following are equivalent:*

(1) *X is a tight $\mathcal{S}$-code.*

(2) *X is a tight $\mathcal{S}*\mathcal{S}$-design.*

(3) *X is an $\mathcal{S}$-code and an $\mathcal{S}*\mathcal{S}$-design.*

An $\mathcal{S}*\mathcal{S}$-design satisfies that $|X| \geq \sum_{(k,l)\in\mathcal{S}} \dim(\mathrm{Harm}(k,l))$, and an $\mathcal{S}*\mathcal{S}$-design X is *tight* if the equality is attained.

Let X have an angle set $D(X) = \{\alpha_1,\dots,\alpha_s\}$, and set $\alpha_0 = 1$. For $0 \leq i \leq s$, define the binary relation R_i as the set of pairs $(\boldsymbol{x},\boldsymbol{y}) \in X \times X$ such that $\boldsymbol{x}^*\boldsymbol{y} = \alpha_i$. The following is a key theorem to characterize tight 3-codes.

Theorem 12 ([23, Theorem 6.1])**.** *Let X be a tight $\mathcal{S}$-design with degree $s = |\mathcal{S}|-1$ for a lower set $\mathcal{S}$. Then X with binary relations defined from angles is a commutative association scheme. Moreover, the primitive idempotents are $\frac{1}{|X|}\boldsymbol{H}_{k,l}\boldsymbol{H}_{k,l}^*$, $(k,l) \in \mathcal{S}$.*

Remark 5. If X is a finite set in $\Omega(d)$, then the Gram matrix $\boldsymbol{G} = (\boldsymbol{x}^*\boldsymbol{y})_{\boldsymbol{x},\boldsymbol{y}\in X}$ is $\frac{1}{d}\boldsymbol{H}_{0,1}\boldsymbol{H}_{0,1}^*$.

To characterize the tight 3-codes, we use the theory of commutative association schemes.

Let X be a finite set and let R_i be a nonempty binary relation on X for $i \in \{0,1,\dots,s\}$. The *adjacency matrix* $\boldsymbol{A}_i$ of relation R_i is defined to be the $(0,1)$-matrix with rows and columns indexed by X such that $(\boldsymbol{A}_i)_{xy} = 1$ if $(x,y) \in R_i$ and $(\boldsymbol{A}_i)_{xy} = 0$ otherwise. A pair $(X, \{R_i\}_{i=0}^s)$ is a *commutative association scheme*, or simply an *association scheme* if the following five conditions hold:

(1) $\boldsymbol{A}_0$ is the identity matrix.

(2) $\sum_{i=0}^s \boldsymbol{A}_i = \boldsymbol{J}$, where $\boldsymbol{J}$ is the all-one matrix.

(3) For any $i \in \{0, 1, \ldots, s\}$, there exists $i' \in \{0, 1, \ldots, s\}$ such that $\boldsymbol{A}_i^T = \boldsymbol{A}_{i'}$.

(4) For any $i, j, k \in \{0, 1, \ldots, s\}$, there exists $p_{i,j}^k$ such that $\boldsymbol{A}_i \boldsymbol{A}_j = \sum_{k=0}^{s} p_{i,j}^k \boldsymbol{A}_k$.

(5) $\boldsymbol{A}_i \boldsymbol{A}_j = \boldsymbol{A}_j \boldsymbol{A}_i$ for any i, j.

The algebra $\mathcal{A}$ generated by all adjacency matrices $\boldsymbol{A}_0, \boldsymbol{A}_1, \ldots, \boldsymbol{A}_s$ over $\mathbb{C}$ is called the *Bose-Mesner algebra*.

Since the Bose-Mesner algebra is semisimple and commutative, there exists a unique set of primitive idempotents of the Bose-Mesner algebra, which is denoted by $\{\boldsymbol{E}_0, \boldsymbol{E}_1, \ldots, \boldsymbol{E}_s\}$ [3, Theorem 3.1]. Since $\{\boldsymbol{E}_0^T, \boldsymbol{E}_1^T, \ldots, \boldsymbol{E}_s^T\}$ forms also the set of primitive idempotents, we define $\hat{i}$ by the index such that $\boldsymbol{E}_{\hat{i}} = \boldsymbol{E}_i^T$ for $0 \leq i \leq s$. Note that $\hat{0} = 0$. The Bose-Mesner algebra is closed under the entrywise product $\circ$. We define structure constants, the *Krein parameters* $q_{i,j}^k$, for $\boldsymbol{E}_0, \boldsymbol{E}_1, \ldots, \boldsymbol{E}_s$ under entrywise product:

$$|X|\boldsymbol{E}_i \circ |X|\boldsymbol{E}_j = |X| \sum_{k=0}^{s} q_{i,j}^k \boldsymbol{E}_k.$$

By the commutativity of the entrywise product, $q_{i,j}^k = q_{j,i}^k$ holds for any i, j. We need the following fundamental properties on Krein parameters in the proof of Theorem 14.

Lemma 13. *Let $(X, \{R_i\}_{i=0}^s)$ be a commutative association scheme of class s. Let $q_{i,j}^k$ be its Krein parameters. Then the following hold for any i, j, k, l.*

(1) $q_{i,j}^k \geq 0$.

(2) $q_{i,0}^k = \delta_{i,k}$.

(3) $q_{i,j}^0 = m_i \delta_{i,\hat{j}}$.

(4) $\sum_{j=0}^{s} q_{i,j}^k = m_i$.

(5) $m_k q_{i,j}^k = m_{\hat{j}} q_{i,\hat{k}}^{\hat{j}}$.

(6) $\sum_{\alpha=0}^{s} q_{i,j}^{\alpha} q_{k,\alpha}^{l} = \sum_{\beta=0}^{s} q_{k,i}^{\beta} q_{\beta,j}^{l}$.

Proof. See [3, Proposition 3.7, Theorem 3.8]. $\square$

The matrix $\boldsymbol{B}_i^* = (q_{i,j}^k)_{j,k=0}^s$ is called the *Krein matrix* for $i \in \{0, 1, \ldots, s\}$.

Both sets of matrices $\{\boldsymbol{A}_0, \boldsymbol{A}_1, \ldots, \boldsymbol{A}_s\}$ and $\{\boldsymbol{E}_0, \boldsymbol{E}_1, \ldots, \boldsymbol{E}_s\}$ are bases for the Bose-Mesner algebra. Therefore there exist change of basis matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ defined as follows;

$$\boldsymbol{A}_i = \sum_{j=0}^{s} \boldsymbol{P}_{ji} \boldsymbol{E}_j, \quad \boldsymbol{E}_j = \frac{1}{|X|} \sum_{i=0}^{s} \boldsymbol{Q}_{ij} \boldsymbol{A}_i.$$

Then we have $\boldsymbol{P} = \frac{1}{|X|}\boldsymbol{Q}^{-1}$. We call $\boldsymbol{P}$ and $\boldsymbol{Q}$ the *eigenmatrix* and *second eigenmatrix* of the association scheme, respectively. For each $i \in \{0, 1, \ldots, s\}$, $k_i := \boldsymbol{P}_{i0}$ and $m_i := \boldsymbol{Q}_{i0}$ are called the i-th valency and multiplicity, respectively.

The Krein matrices $\boldsymbol{B}_i^*$ and the second eigenmatrix $\boldsymbol{Q}$ are related as follows. The proof is essentially same as that of [3, Theorem 4.1]. A vector $\boldsymbol{v}$ is *standard* if the first entry of $\boldsymbol{v}$ is 1.

Lemma 14. *Let $(X, \{R_i\}_{i=0}^s)$ be a commutative association scheme with the Krein matrices $\boldsymbol{B}_i^*$ and the second eigenmatrix $\boldsymbol{Q}$. Let $\boldsymbol{v}_i = (\boldsymbol{Q}_{i0}, \boldsymbol{Q}_{i1}, \ldots, \boldsymbol{Q}_{is})$ be the i-th row of $\boldsymbol{Q}$ for $i \in \{0, 1, \ldots, s\}$. Then $\boldsymbol{v}_i^T$ is characterized as the unique standardized common right eigenvector $\boldsymbol{v}^T$ of the Krein matrices $\boldsymbol{B}_j^*$ such that $\boldsymbol{B}_j^* \boldsymbol{v}^T = \boldsymbol{Q}_{ij}\boldsymbol{v}^T$.*

Proof. Regard the left multiplication with respect to the entrywise product $\circ$ as linear transformation and express them in matrix form with respect to $\{\boldsymbol{E}_0, \boldsymbol{E}_1, \ldots, \boldsymbol{E}_s\}$. Then we have an algebra homomorphism φ from the Bose-Mesner algebra to $\mathrm{Mat}_{s+1}(\mathbb{C})$ defined by $\varphi(\boldsymbol{E}_i) = (\boldsymbol{B}_i^*)^T$. The rest of the proof is obtained by replacing the roles $\boldsymbol{A}_i, \boldsymbol{P}$ with $\boldsymbol{E}_i, \boldsymbol{Q}$ respectively in the proof of [3, Theorem 4.1(ii)]. $\square$

We mention that a complex spherical s-code can be obtained from a commutative association scheme of class s as follows. Let $\boldsymbol{E}_i$ be a primitive idempotent of the commutative association scheme such that $\boldsymbol{E}_i^T \neq \boldsymbol{E}_i$ and $\boldsymbol{E}_i$ has no repeated rows. Since the primitive idempotent is positive semidefinite Hermitian matrices, there exists a $|X| \times m_i$ matrix $\boldsymbol{F}$ such that $\boldsymbol{F}\boldsymbol{F}^T = (1/m_i|X|)\boldsymbol{E}_i$. Then the set X of the column vectors of $\boldsymbol{F}$ forms a finite set in $\Omega(m_i)$ such that $D(X) = \{\boldsymbol{Q}_{ji}/\boldsymbol{Q}_{0i} \mid 1 \leq j \leq s\}$. We give an example of complex 3-codes in this manner. This example is not tight, but has large cardinality.

Example 1. In [11], an infinite family of certain distance-regular digraphs of girth 4 was constructed. Note that a distance-regular digraph of girth $s+1$ corresponds to a commutative association scheme of class s with the adjacency matrices determined from the path length in digraphs [6]. The commutative association scheme of class 3 has the following second eigenmatrix [8]:

$$\boldsymbol{Q} = \begin{pmatrix} 1 & \mu(2\mu^2-1) & (2\mu^2-1)(2\mu^2-2\mu+1) & \mu(2\mu^2-1) \\ 1 & \mu^2-\mu+\mu^2\sqrt{-1} & -(2\mu^2-2\mu+1) & \mu^2-\mu-\mu^2\sqrt{-1} \\ 1 & -\mu & 2\mu-1 & -\mu \\ 1 & \mu^2-\mu-\mu^2\sqrt{-1} & -(2\mu^2-2\mu+1) & \mu^2-\mu+\mu^2\sqrt{-1} \end{pmatrix},$$

where μ is any power of 2. Then the primitive idempotent $\boldsymbol{E}_1$ yields a complex spherical 3-code X in $\Omega(\mu(2\mu^2-1))$ with $|X| = 4\mu^4$ and

$$D(X) = \left\{ \frac{\mu - 1 \pm \mu\sqrt{-1}}{2\mu^2-1}, \frac{-1}{2\mu^2-1} \right\}.$$

6.1 Tight complex spherical 3-codes

Let X be a 3-code in $\Omega(d)$ with $D(X) = \{\alpha, \overline{\alpha}, \beta\}$, where α is an imaginary number and β is a real number. Note that $\phi(X)$ is a real s-code with $s = 1$ or 2. When $d = 1$, $|X| = |\phi(X)| \leq 5$ with equality if and only if $\phi(X)$ is the regular 5-gon [7]. In this case, X has the following angle set $\{e^{2\pi i/5} : 0 \leq i \leq 4\}$, which implies that X has degree 4. Thus $|X| \leq 4$ holds. When $d \geq 2$, we can easily find real numbers a, b, c such that $F(x) = ax\overline{x} + b(x + \overline{x}) + c$ is an annihilator polynomial of X. This implies that X is an $\mathcal{S}$-code, where $\mathcal{S} = \{(0, 0), (1, 0), (0, 1), (1, 1)\}$. By Theorem 10 with equation (12), we have the following upper bound for 3-codes.

Theorem 13. *Let X be a 3-code in $\Omega(d)$. Then*

$$|X| \leq \begin{cases} 4 & \textit{if } d = 1, \\ d^2 + 2d & \textit{if } d \geq 2. \end{cases}$$

Note that the example for $d = 1$ coincides with the case of $\mu = 1$ in Example 1. However, a tight 3-code is rare, shown in the following theorem.

Theorem 14. *Let X be a 3-code in $\Omega(d)$ attaining equality in Theorem 13. Then one of the following holds;*

(1) $d = 1$ *and* $D(X) = \{\pm\sqrt{-1}, -1\}$,

(2) $d = 2$ *and* $D(X) = \{\pm\sqrt{-1}/\sqrt{3}, -1\}$.

Proof. Let X be a tight 3-code in $\Omega(1)$ with $D(X) = \{\alpha, \overline{\alpha}, \beta\}$. After the unitary operation, we may assume that $1 \in X$. Then $X = \{1, \alpha, \overline{\alpha}, \beta\}$. Since β is a real number, $\beta = -1$. Then $\alpha = \sqrt{-1}$ as desired.

Let d be an integer at least 2. Since X is a tight $\mathcal{S}$-code, X is an $\mathcal{S} * \mathcal{S}$-design by Theorem 11. Since the degree of X is 3, X with the binary relations obtained from the angles of X carries a commutative association scheme by Theorem 12. Then the Gram matrix of X is a scalar multiple of some primitive idempotent of the association scheme, say $\boldsymbol{E}_1$. And we arrange the ordering of the primitive idempotents so that $\boldsymbol{E}_2 = \boldsymbol{E}_1^T$ holds and $\boldsymbol{E}_3$ is a real matrix. Then $\hat{1} = 2, \hat{2} = 1, \hat{3} = 3$ hold.

We will determine the Krein matrix $\boldsymbol{B}_1^*$ and the second eigenmatrix $\boldsymbol{Q}$. We use Lemma 13 (2),(3) to obtain $q_{1,0}^0 = q_{1,0}^2 = q_{1,0}^3 = q_{1,1}^0 = q_{1,3}^0 = 0$, $q_{1,0}^1 = 1$, and $q_{1,2}^0 = d$. By Theorem 12, we may set

$$\boldsymbol{E}_1 = \frac{1}{|X|}\boldsymbol{H}_{1,0}\boldsymbol{H}_{1,0}^*,$$

$$\boldsymbol{E}_2 = \frac{1}{|X|}\boldsymbol{H}_{0,1}\boldsymbol{H}_{0,1}^*,$$

$$\boldsymbol{E}_3 = \frac{1}{|X|}\boldsymbol{H}_{1,1}\boldsymbol{H}_{1,1}^*.$$

By the recurrence (13), we have that $\boldsymbol{E}_2 = \frac{1}{|X|} g_{0,1} \circ (\frac{|X|}{d} \boldsymbol{E}_1)$ and $\boldsymbol{E}_3 = \frac{1}{|X|} g_{1,1} \circ (\frac{|X|}{d} \boldsymbol{E}_1)$, where $f \circ (\boldsymbol{M})$ denotes the matrix obtained by applying a function f to each entry of a matrix $\boldsymbol{M}$. By the recurrence (13) of the Jacobi polynomial, the Krein parameters $q_{1,2}^1, q_{1,2}^2, q_{1,2}^3$ are the same as the coefficients of the Jacobi polynomials in the product $g_{1,0}(x) g_{0,1}(x)$, namely $q_{1,2}^1 = q_{1,2}^2 = 0$ and $q_{1,2}^3 = \frac{d}{d+1}$ holds. Since X is an $\mathcal{S} * \mathcal{S}$-design and $\mathcal{S} * \mathcal{S}$ contains $(2,1)$, $q_{1,1}^1 = 0$ holds by [23, Corollary 9.3 (ii)]. By Lemma 13 (4), we have

$$q_{1,1}^2 + q_{1,3}^2 = d, \tag{15}$$

$$q_{1,1}^3 + q_{1,3}^3 = \frac{d^2}{d+1}. \tag{16}$$

We have $m_1 = \dim(\mathrm{Harm}(1,0)) = d$ and $m_3 = \dim(\mathrm{Harm}(1,1)) = d^2 - 1$ by (12). Substituting the values m_1, m_3 into the equation in Lemma 13 (5) for $(i,j,k) = (1,1,3)$, we have

$$(d^2 - 1) q_{1,1}^3 = d q_{1,3}^2. \tag{17}$$

Using the equation in Lemma 13 (6) for $(i,j,k,l) = (1,1,2,1)$, we have

$$(q_{1,1}^2)^2 + \frac{d^2-1}{d} q_{1,1}^3 q_{1,3}^2 = \frac{2d^2}{d+1}. \tag{18}$$

We solve the equations (15)–(18) to obtain

$$(q_{1,1}^2, q_{1,1}^3, q_{1,3}^2, q_{1,3}^3) = \begin{cases} \left(\frac{d(d-(d-1)\sqrt{d+2})}{d^2+d-1}, \frac{d^2(d+1+\sqrt{d+2})}{(d+1)(d^2+d-1)}, \frac{d(d-1)(d+1+\sqrt{d+2})}{d^2+d-1}, \frac{d^2(d^2-2-\sqrt{d+2})}{(d+1)(d^2+d-1)}\right), \\ \left(\frac{d(d+(d-1)\sqrt{d+2})}{d^2+d-1}, \frac{d^2(d+1-\sqrt{d+2})}{(d+1)(d^2+d-1)}, \frac{d(d-1)(d+1-\sqrt{d+2})}{d^2+d-1}, \frac{d^2(d^2-2+\sqrt{d+2})}{(d+1)(d^2+d-1)}\right). \end{cases} \tag{19}$$

First we consider the former case in (19). Since the Krein number $q_{1,1}^2$ is nonnegative by Lemma 13 (1), we must have $d = 2$. In this case the second eigenmatrix $\boldsymbol{Q}$ is given by Lemma 14 as

$$\boldsymbol{Q} = \begin{pmatrix} 1 & 2 & 2 & 3 \\ 1 & \frac{2\sqrt{-1}}{\sqrt{3}} & -\frac{2\sqrt{-1}}{\sqrt{3}} & -1 \\ 1 & -\frac{2\sqrt{-1}}{\sqrt{3}} & \frac{2\sqrt{-1}}{\sqrt{3}} & -1 \\ 1 & -2 & -2 & 3 \end{pmatrix}.$$

Thus we have that X is a complex 3-code with $D(X) = \{\pm\sqrt{-1}/\sqrt{3}, -1\}$.

Next, in the latter case in (19), we set $t = \sqrt{d+2}$. The second eigenmatrix is given by Lemma 14 as

$$\boldsymbol{Q} = \begin{pmatrix} 1 & t^2 - 2 & t^2 - 2 & (t^2-3)(t^2-1) \\ 1 & \frac{t^2-2}{t+1} & \frac{t^2-2}{t+1} & 1 - 2t + \frac{2}{t+1} \\ 1 & \frac{(t^2-2)(t^2+t-1+t\sqrt{-3t^2-2t+5})}{2(t^3-2t+1)} & \frac{-6-3t+3t^2+2t^3-t\sqrt{-3t^2-2t+5}}{4(t^2-1)(t^2+t-1)} & \frac{(t+1)(t^2-3)}{t^2+t-1} \\ 1 & \frac{-6-3t+3t^2+2t^3-t\sqrt{-3t^2-2t+5}}{4(t^2-1)(t^2+t-1)} & \frac{(t^2-2)(t^2+t-1+t\sqrt{-3t^2-2t+5})}{2(t^3-2t+1)} & \frac{(t+1)(t^2-3)}{t^2+t-1} \end{pmatrix}.$$

Then the valency corresponding to the second row of the second eigenmatrix is determined as $k_1 = \frac{(t+1)^3(t^2-3)}{3t+5}$ by $\boldsymbol{P} = \frac{1}{|X|}\boldsymbol{Q}^{-1}$. By substituting $t = \sqrt{d+2}$, we find that the valency k_1 is equal to $\frac{(d-1)(3d^2+6d-5+4(d-1)\sqrt{d+2})}{9d-7}$, which implies that $t = \sqrt{d+2}$ must be an integer. The partial fraction decomposition $243k_1 = 81t^4 + 108t^3 - 180t^2 - 348t - 149 + \frac{16}{3t+5}$ shows that $3t+5$ divides 16. Since t is positive, we have $t = 1$ and thus $d = -1$. This contradicts to the fact that d is positive. $\square$

For $d = 1, 2$, the tight 3-code is unique, that is proved in Section 5. The tight 3-code in $\Omega(1)$ is $X = \{\pm 1, \pm\sqrt{-1}\}$. The tight 3-code in $\Omega(2)$ is $\{\pm x_1, \pm x_2, \pm x_3, \pm x_4\}$, where $x_1 = (1, 0)$, $x_2 = 1/\sqrt{6}(\sqrt{-2}, 1 + \sqrt{-3})$, $x_3 = 1/\sqrt{6}(\sqrt{-2}, 1 - \sqrt{-3})$, $x_4 = 1/\sqrt{6}(\sqrt{-2}, -2)$.

Remark 6. For $\mathcal{S} = \{(0,0),(1,0),(0,1),(1,1)\}$, the tight $\mathcal{S}$-codes with degree 4 were given in [23, Example 10.2]. They are obtained from the subconstituents of SIC-POVMs in dimension $d = 2, 8$. SIC-POVMs are the tight projective 1-codes, see [21] more details.

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