Complex Spherical Codes with Three Inner Products

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Abstract
Let $X$ be a finite set in a complex sphere of dimension $d$. Let $D(X)$ be the set of usual inner products of two distinct vectors in $X$. 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 wish to classify the largest possible $s$-codes for a given dimension $d$. In this paper, we consider the problem for the case $s = 3$. In an earlier work, Roy and Suda (J Comb Des 22(3):105–148, 2014) gave certain upper bounds for the cardinality of a 3-code. 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. Further, we construct an algorithm to classify the largest 3-codes by considering representations of oriented graphs. With this algorithm, we are able to classify the largest 3-codes for dimensions 1, 2, 3 using a standard computer.

Keywords Complex spherical $s$-code · $s$-Distance set · Tight design · Extremal set theory · Graph representation · Association scheme

Mathematics Subject Classification 05C62 · 05B20

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 as

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

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where \( x^* \) is the conjugate transpose of a column vector \( x \). 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 tight if \( X \) has the largest possible cardinality in all \( s \)-codes in \( \Omega(d) \). One major problem for \( s \)-codes is classifying the largest \( s \)-codes for given \( s \) and \( d \).

For the real unit sphere \( S^{d-1} \), a similar concept to \( s \)-codes has been well studied [7]. A subset \( X \) of \( S^{d-1} \) is an \( s \)-distance set if \( |D(X)| = s \). Delsarte et al. [7] gave an upper bound for an \( s \)-distance set \( X \) in \( S^{d-1} \). A \( s \)-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 for all but \( s = 2 \) [1, 2, 4, 16]. The largest 1-distance set in \( S^{d-1} \) is the regular simplex, and 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 \( d = (2k + 1)^2 - 3 \), with \( k \in \mathbb{N} \) [5, 10, 12, 14]. 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 for all \((s, d)\) 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 \( \Omega(d) \) [20, 23]:

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

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 having no symmetric pair of directed edges. An oriented graph \( G = (V, E) \) is representable in \( \Omega(d) \) if there exists a mapping \( \varphi \) from \( V \) to \( \Omega(d) \), an imaginary number \( \alpha \) with \( \text{Im}(\alpha) > 0 \), and a real number \( \beta \) such that for any \( u, v \in V \),
The image of the map \( \phi \) 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 \( A \) be the adjacency matrix of \( G \). The Gram matrix \( H \) of a complex spherical representation of \( G \) can be expressed by

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

for some real number \( c \) and some real matrix \( M \). Actually, \( M \) is positive semidefinite. The matrix \( M \) can be identified with a real spherical representation of a simple graph \( G' \) whose adjacency matrix is \( A + A^T \). The dimension of a real spherical representation is studied in [8,18,22]. Results related to real representations are helpful for determining the dimension of a complex spherical representation. In this paper, we construct 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 Sect. 2, we collect known results of Euclidean representations of a simple graph. In Sect. 3, we show several results for Hermitian matrices used to determine the dimensions of complex representations, and we consider the dimension of a complex representation of an oriented graph in Sect. 4. In Sect. 5, we present 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 Sect. 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 real representations 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 \( A \) of \( G \) is the matrix indexed by \( V \), with entries

\[
A_{xy} = \begin{cases} 
1 & \text{if } (x, y) \in E, \\
0 & \text{otherwise}.
\end{cases}
\]

Suppose that \( G \) is simple and is not a complete graph or a union of isolated vertices. Let \( A \) be the adjacency matrix of \( G \), and \( \overline{A} \) that of the complement. The matrix \( M_c \) is defined as

\[
M_c = cA + \overline{A}
\]

for a real number \( c \) such that \( 0 \leq c < 1 \). 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 \( M_c \) of \( G \) for some
Theorem 2.1 [8] Let G be a simple graph, and let \( M_e \) and \( \text{Rep}(G) \) be defined as above. There then exists \( \xi \in \mathbb{R} \) such that 0 ≤ \( \xi \) < 1, and the following conditions hold:

1. \( M_\xi \) is the distance matrix in \( \text{Rep}(G) \) dimension.
2. For \( \xi < c < 1 \), \( M_e \) is the distance matrix in \( n - 1 \) dimension, and not in \( n - 2 \) dimension.
3. For 0 ≤ \( c < \xi \), \( M_e \) 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 \( M_\xi \), where \( \xi \) is given in Theorem 2.1. Roy [22] determined \( \text{Rep}(G) \) by eigenvalues and eigenspaces of the adjacency matrix of \( G \). Let \( j \) be the all-ones column vector.

Theorem 2.2 [22, Lem. 4,5,6, Thm. 7] Let \( G \) be a simple graph with adjacency matrix \( A \). Let \( \lambda_i \) be the \( i \)-th smallest distinct eigenvalue of \( A \), \( m_i \) the multiplicity of \( \lambda_i \), and \( E_i \) the eigenspace corresponding to \( \lambda_i \). Let \( P_i \) be the orthogonal projection matrix onto \( E_i \). Let \( \beta_i \) be the main angle of \( \lambda_i \), namely, \( \beta_i = \sqrt{(P_i \cdot j) \cdot (P_i \cdot j) / n} \). Then the following conditions hold:

1. If \( \beta_1 = 0 \), then \( \xi = (\lambda_1 + 1) / \lambda_1 \) and \( \text{Rep}(G) = n - m_1 - 1 \).
2. If \( \beta_1 \neq 0 \) and \( m_1 > 1 \), then \( \xi = (\lambda_1 + 1) / \lambda_1 \) and \( \text{Rep}(G) = n - m_1 \).
3. If \( \beta_2 = 0 \), \( m_1 = 1 \), \( \lambda_2 < -1 \), and \( \beta_1^2 / (\lambda_2 - \lambda_1) = \sum_{i \geq 3} \beta_i^2 / (\lambda_i - \lambda_2) \), then \( \xi = (\lambda_2 + 1) / \lambda_2 \) and \( \text{Rep}(G) = n - m_2 - 2 \).
4. If \( \beta_2 = 0 \), \( m_1 = 1 \), \( \lambda_2 < -1 \), and \( \beta_1^2 / (\lambda_2 - \lambda_1) > \sum_{i \geq 3} \beta_i^2 / (\lambda_i - \lambda_2) \), then \( \xi = (\lambda_2 + 1) / \lambda_2 \) and \( \text{Rep}(G) = n - m_2 - 1 \).
5. Otherwise, we have \( \xi < (\lambda_1 + 1) / \lambda_1 \), \( \xi \neq (\lambda_2 + 1) / \lambda_2 \) and \( \text{Rep}(G) = n - 2 \).

A graph \( G \) is of Type (i) if \( G \) satisfies condition (i) from Theorem 2.2 for \( i \in \{1, \ldots, 5\} \). A Euclidean representation \( X \) of \( G \) is spherical if \( X \) can be on a sphere.

Theorem 2.3 [18] Let \( G \) be a simple graph. Then the following conditions 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 2.1 is spherical.

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

Lemma 2.4 [17] If \( M \) is a dissimilarity matrix, then the following are equivalent:

1. \( M \) is a distance matrix of embedding dimension \( d \).
2. \( -PMMP \) is a positive semidefinite matrix of rank \( d \).

Lemma 2.5 [17] If \( M \) is a dissimilarity matrix, then the following are equivalent:
(1) There uniquely exists $a \in \mathbb{R}$ such that $a > 0$, $-M + aJ$ is a positive semidefinite matrix of rank $d$, $-M + a'J$ is a positive semidefinite matrix of rank $d + 1$ for $a' > a$, and $-M + cJ$ is not positive semidefinite for $c < a$.

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

### 3 Results for Hermitian Matrices

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

**Theorem 3.1** [20] Let $H$ be a Hermitian matrix, and $M = H + aJ$ for a real number $a$. Let $\tau_1, \ldots, \tau_r$ be the distinct main eigenvalues of $H$ such that $\tau_1 < \tau_2 < \cdots < \tau_r$. Let $\mu_1, \ldots, \mu_s$ be the distinct main eigenvalues of $M$ such that $\mu_1 < \mu_2 < \cdots < \mu_s$. Let $\beta_i$ be the main angle of $\tau_i$. Then $r = s$ holds, and

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

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 3.2** Let $H$ be a Hermitian matrix of size $n$. Let $\tau_1, \ldots, \tau_r$ be the distinct main eigenvalues of $H$ such that $\tau_1 < \tau_2 < \cdots < \tau_r$. Let $\beta_i$ be the main angle of $\tau_i$. Let $P$ be the orthogonal projection matrix onto $j^\perp$, namely $P = I - (1/n)J$. If $H$ is not positive semidefinite, then the following are equivalent:

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

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

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

$(1) \Rightarrow (2)$: Since $H + aJ$ is positive semidefinite, we have $\lambda = v^*Hv = v^*P(H + aJ)Pv \geq 0$. Since $H$ is not positive semidefinite, we have $\tau_1 < 0$. Let $\mu_1, \ldots, \mu_r$ be the distinct main eigenvalues of $H + aJ$ such that $\mu_1 < \mu_2 < \cdots < \mu_r$. By Theorem 3.1, we have $\tau_1 < \mu_1 < \tau_2$. Since $H + aJ$ is positive semidefinite, we have $0 \leq \mu_1 < \tau_2$. By (1) for $x = 0$, it follows that $\sum_{i=1}^{r} n\beta_i^2/\tau_i < 0$ and $a \geq -1/\left(\sum_{i=1}^{r} n\beta_i^2/\tau_i\right)$. In particular, $\mu_1 = 0$ if and only if $a = -1/\left(\sum_{i=1}^{r} n\beta_i^2/\tau_i\right) > 0$. Since $H + aJ$ is positive semidefinite, so is $P(H + aJ)P = PHP$.  

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(2) ⇒ (1): Since \( v \) is orthogonal to the all-ones vector and \( PHP \) is positive semidefinite, we have

\[
\lambda = v^* H v = v^* PHP v \geq 0.
\]  

(2)

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

We can verify the following remarks by the proof of Lemma 3.2.

**Remark 3.3** If Lemma 3.2 (1) holds, then

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

**Remark 3.4** If Lemma 3.2 (2) holds, then the null space of \( H \) is contained in \( j \perp \).

**Remark 3.5** If Lemma 3.2 (2) holds, then \( \text{Rank}(H + aJ) = \text{Rank}(PHP) \) for \( a = -1/(\sum_{i=1}^r n \beta_i^2 / \tau_i) \).

**Theorem 3.6** Let \( H \) be a Hermitian matrix. Let \( M \) and \( A \) be the real matrices such that \( H = M + \sqrt{-1}A \). Let \( E_0 \) be the null space of \( \sqrt{-1}A \), and \( E' \) the null space of \( M \). If \( H \) is positive semidefinite, then \( E'_0 \subseteq E_0 \) holds.

**Proof** Since \( M \) is a real symmetric matrix, we can take a basis of \( E'_0 \) consisting of real vectors. For a real vector \( v \in E'_0 \), we have

\[
v^* H v = v^* M v + \sqrt{-1} v^* A v = 0
\]

because \( A \) is skew-symmetric. Since \( H \) is positive semidefinite, \( v^* H v = 0 \) if and only if \( H v = o \). It thus follows that

\[
o = H v = M v + \sqrt{-1} A v = \sqrt{-1} A v.
\]

Therefore, \( E'_0 \subseteq E_0 \) holds.

**Theorem 3.7** Let \( H \) be a Hermitian matrix. Let \( M \) and \( A \) be the real matrices such that \( H = M + \sqrt{-1}A \). If \( H \) is positive semidefinite, then \( 2 \text{Rank}(H) \geq \text{Rank}(M) \).

**Proof** By Theorem 3.6, we have \( E'_0 \subseteq E_0 \). Let \( E_+ \) (resp. \( E_- \)) be the direct sum of eigenspaces corresponding to the positive (resp. negative) eigenvalues of \( \sqrt{-1}A \). It is easily proved that \( \dim E_+ = \dim E_- \). For a non-zero vector \( v \in E_+ \oplus ((E'_0) \perp \cap E_0) \), we have \( v^* H v > 0 \) because \( M \) is positive semidefinite. Therefore,

\[
\text{Rank}(H) \geq \dim(E_+ \oplus ((E'_0) \perp \cap E_0))
\]

\[
= \dim(E_+) + \dim((E'_0) \perp \cap E_0)
\]

\[
= \dim(E_+) + \dim((E'_0) \perp) + \dim(E_0) - \dim((E'_0) \perp \cap E_0)
\]
\[
\begin{align*}
&= \frac{1}{2} \text{Rank}(A) + \text{Rank}(M) + (n - \text{Rank}(A)) - n \\
&= \text{Rank}(M) - \frac{1}{2} \text{Rank}(A) \\
&\geq \text{Rank}(M) - \frac{1}{2} \text{Rank}(M) \\
&= \frac{1}{2} \text{Rank}(M),
\end{align*}
\]

where \( n \) is the size of \( H \). Thus the theorem follows. \( \square \)

**Theorem 3.8** Let \( H \) be a Hermitian matrix. Let \( M \) and \( A \) be the real matrices such that \( H = M + \sqrt{-1}A \). Let \( \mathcal{E}_0 \) be the null space of \( \sqrt{-1}A \). Let \( \mathcal{E}_0' \) be the null space of \( M \). Suppose \( M \) is positive semidefinite, and \( \mathcal{E}_0' \subset \mathcal{E}_0 \) holds. Then there exists a unique \( \eta > 0 \) such that the following conditions hold:

1. \( M + \eta \sqrt{-1}A \) is positive semidefinite, and its rank is smaller than \( \text{Rank}(M) \).
2. \( M + c \sqrt{-1}A \) is positive semidefinite for \( 0 \leq c < \eta \), and its rank is equal to \( \text{Rank}(M) \).
3. \( M + c \sqrt{-1}A \) is not positive semidefinite for \( c < \eta \).

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

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

Note that \( \Phi(c) \geq 0 \) if and only if \( M + c \sqrt{-1}A \) is positive semidefinite, and \( \text{Rank}(M + c \sqrt{-1}A) \leq \text{Rank}(M) \). In particular, \( \Phi(c) = 0 \) if and only if \( \text{Rank}(M + c \sqrt{-1}A) < \text{Rank}(M) \). Since \( \Phi(c) \) is the minimum value of the collection of linear functions in \( c \), the function \( \Phi(c) \) is concave. Since \( M \) is positive semidefinite, we have \( \Phi(0) > 0 \). There exists \( v \in (\mathcal{E}_0')^\perp \) such that \( v^* (\sqrt{-1}A)v < 0 \). 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 \( D(X) = \{\alpha, \alpha, \beta\} \), where \( \alpha \) is an imaginary number with \( \text{Im}(\alpha) > 0 \), and \( \beta \in \mathbb{R} \). Let \( E = \{(x, y) \in X \times X \mid x^*y = \alpha\} \), and \( E' = \{(x, y) \mid (x, y) \in E \text{ or } (y, x) \in E\} \). Let \( G \) be the oriented graph \( (X, E) \) with adjacency matrix \( A \), and \( G' \) the simple graph \( (X, E') \) with adjacency matrix \( B \). Let \( \overline{B} \) be the adjacency matrix of the complement of \( G' \). The Gram matrix \( H \) of a complex spherical representation of \( G \) can be expressed by

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

for a real number \( c \) and a real matrix \( M \). Let \( \phi \) 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 $\psi(x)^T \psi(y) = \text{Re}(x^* y)$ for $x, y \in \Omega(d)$. The matrix $M$ is the Gram matrix of \( \psi(X) = \{ \psi(x) \mid x \in X \} \). The representation $\psi(X)$ of $G'$ is spherical. By Lemma 2.5, $M$ can be expressed by

$$M = -(bB + \overline{B}) + aJ$$

for $a > 0$ and $b \geq 0$. Note that $bB + \overline{B}$ is the distance matrix of $\psi(X)$ after rescaling the two distances to 1 and $b$. Since $\psi(X)$ is spherical, $\psi(X)$ is the minimal representation of $G'$ of Type (1), (2), or (4), or a non-minimal representation by Theorem 2.3.

By Theorem 3.6, the null space $E'_0$ of $M$ must be contained in the null space $E_0$ of $\sqrt{-1}(A - A^T)$. When we consider a minimal-dimensional representation of a given oriented graph $G$, the minimal representation of $G'$ rarely satisfies $E'_0 \subseteq E_0$. We give simple examples:

$G_1 : A_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$, $G_2 : A_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$.

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

$$M_1 = -\left( \frac{1}{2} B + \overline{B} \right) + \frac{1}{2} J = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$ 

The null space of $M_1$ is \( \text{Span}\{(1, 0, 1, 0), (0, 1, 0, 1)\} \). This coincides with the null space of $\sqrt{-1}(A_1 - A_1^T)$. Actually, we can give a minimal-dimensional representation in $\Omega(1)$ of $G_1$ as

$$H_1 = -\left( \frac{1}{2} B + \overline{B} \right) + \frac{1}{2} J + \frac{1}{2} \sqrt{-1}(A_1 - A_1^T)$$

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

On the other hand, the eigenvalues of $\sqrt{-1}(A_2 - A_2^T)$ are $\{-\sqrt{2}, -\sqrt{2}, \sqrt{2}, \sqrt{2}\}$, and hence the null space is empty. In this case, $\text{Rank}(M_2)$ must be 4, and we use a non-minimal representation of $G'$:

\[ \text{Springer} \]
Let $G$ be an oriented graph.

**Lemma 4.2** (evaluation of Rank and $3.5$). Therefore, we choose a spherical 3-code in $\Omega_1(n)$, namely $\Omega_1(n)$.

We can then give a minimal-dimensional representation in $\Omega(2)$ of $A_2$ as

$$H_2 = -(B + \overline{B}) + J + \sqrt{- \frac{1}{2}} (A_2 - A_2^T) = \begin{pmatrix} 1 & -\sqrt{-\frac{1}{2}} & 0 & -\sqrt{-\frac{1}{2}} \\ \sqrt{-\frac{1}{2}} & 1 & \sqrt{-\frac{1}{2}} & 0 \\ 0 & -\sqrt{-\frac{1}{2}} & 1 & \sqrt{-\frac{1}{2}} \\ \sqrt{-\frac{1}{2}} & 0 & -\sqrt{-\frac{1}{2}} & 1 \end{pmatrix}.$$  

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 3.7, namely $n \leq 2d + 1$. The union of $d$ triangles that are orthogonal to one another is a spherical 3-code in $\Omega(d)$ and has size $3d$. Therefore, it is sufficient 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 that $G'$ has non-zero $B$ and $\overline{B}$, and $G'$ is of Type (1), (2), or (4). Let $H(a, c)$ denote the matrix defined by

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

for real numbers $a$ and $c$, where $\xi$ is the positive number given in Theorem 2.1. Note that $\xi B + \overline{B}$ is the distance matrix of the minimal representation of $G'$. We wish to determine $a$ and $c$ so that $a > 0$, $c > 0$, $H(a, c)$ is positive semidefinite, and the rank of $H(a, c)$ is minimal. Let $E_0$ be the null space of $\sqrt{-1}(A - A^\top)$, and $E_0'$ be that of $-(\xi B + \overline{B})$.

**Remark 4.1** If $G'$ is of Type (1), (2), or (4), then $E_0' \subset j^\perp$ holds by Lemma 2.5 and Remark 3.4.

Since the diagonal entries in $H(0, c)$ are zero, $H(0, c)$ is not positive semidefinite. If $H(a, c)$ is positive semidefinite, then $H(0, c)$ satisfies condition (2) from Lemma 3.2, and hence $PH(0, c)P$ is positive semidefinite. If $H(0, c)$ satisfies condition (2) from Lemma 3.2, then there exists a unique positive number $a$ such that Rank($H(a, c)$) is minimal, and Rank($H(a, c)$) = Rank($PH(0, c)P$) by Remarks 3.3 and 3.5. Therefore, we choose $c$ so that $PH(0, c)P$ is positive semidefinite, and Rank($PH(0, c)P$) is minimal. The following lemma shows such possible $c$ and the evaluation of Rank($PH(0, c)P$).

**Lemma 4.2** Let $G$ be an oriented graph $(V, E)$ with adjacency matrix $A$. Let $G'$ be the simple graph $(V, E')$ with adjacency matrix $B$, where $E' = \{(u, v) \mid (u, v) \in E')$. 

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E or \((v, u) \in E\). Let \(\overline{B}\) be the adjacency matrix of the complement of \(G'\). Let \(H(a, c)\) be the matrix defined by

\[
H(a, c) = -\left(\xi B + \overline{B}\right) + aJ + c\sqrt{-1}(A - A^T)
\]

for real numbers \(a\) and \(c\), where \(\xi\) is the positive number given in Theorem 2.1. Let \(E_0\) be the null space of \(\sqrt{-1}(A - A^T)\), and \(E'_0\) the null space of \(-\left(\xi B + \overline{B}\right)\). If \(E'_0 \subseteq E_0\) holds, then there exists a unique positive number \(\eta\) such that

(1) \(PH(0, \eta)P\) is positive semidefinite, and

\[
\text{Rank}(PH(0, \eta)P) < \text{Rank}(PH(0, 0)P),
\]

(2) \(PH(0, c)P\) is positive semidefinite, and

\[
\text{Rank}(PH(0, c)P) = \text{Rank}(PH(0, 0)P)
\]

for \(0 < c < \eta\).

(3) \(PH(0, c)P\) is not positive semidefinite for \(\eta < c\).

**Proof** It follows that

\[
PH(0, c)P = -P\left(\xi B + \overline{B}\right)P + c\sqrt{-1}P(A - A^T)P.
\]

It is easily shown that the null space of \(-P\left(\xi B + \overline{B}\right)P\) is contained in that of \(\sqrt{-1}P(A - A^T)P\). This lemma follows from Theorem 3.8.

Next we have to check whether \(H(0, c)\) satisfies condition (2) from Lemma 3.2 for \(0 < c \leq \eta\), where \(\eta\) is the positive number given in Lemma 4.2. If \(H(0, c)\) satisfies condition (2) from Lemma 3.2, we can construct a representation of \(G\) by choosing a suitable number \(a\).

**Theorem 4.3** Let \(G\) be an oriented graph \((V, E)\) with adjacency matrix \(A\). Let \(G'\) be the simple graph \((V, E')\) with adjacency matrix \(B\), 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 \(\overline{B}\) be the adjacency matrix of the complement of \(G'\). Let \(H(a, c)\) be the matrix defined by

\[
H(a, c) = -\left(\xi B + \overline{B}\right) + aJ + c\sqrt{-1}(A - A^T)
\]

for real numbers \(a\) and \(c\), where \(\xi\) is the positive number given in Theorem 2.1. Let

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

and

\[
\text{Rep}(G) = \min\{\text{Rank}(H(a, c)) \mid (a, c) \in U\}.
\]
Let \( \text{Rep}(G') \) be the dimension of the minimal representation of \( G' \). Let \( \mathcal{E}_0 \) be the null space of \( \sqrt{-1}(A - A^T) \), and \( \mathcal{E}_0' \) the null space of \( -(\xi B + \bar{B}) \). Let \( \eta \) be a positive number given in Lemma 4.2. If \( \mathcal{E}_0' \subseteq \mathcal{E}_0 \) holds, then the following conditions hold:

1. If \( H(0, \eta) \) satisfies condition (1) from Lemma 3.2, then
   \[
   \text{Rep}(G) = \text{Rank}(H(0, \eta)) - 1 < \text{Rep}(G').
   \]

2. If \( H(0, \eta) \) does not satisfy condition (1) from Lemma 3.2, then
   \[
   \text{Rep}(G) = \text{Rank}(H(0, 0)) - 1 = \text{Rep}(G').
   \]

**Proof** Since the minimal representation of \( G' \) is spherical, there exists a unique \( a' \in \mathbb{R} \) such that \( H(a', 0) \) is positive semidefinite and \( \text{Rep}(G') = \text{Rank}(H(a', 0)) \) by Lemma 2.5. By Remark 3.5, it follows that \( \text{Rank}(H(a', 0)) = \text{Rank}(PH(0, 0)P) \), and hence

\[
\text{Rep}(G') = \text{Rank}(PH(0, 0)P). \tag{4}
\]

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

\[
\text{Rank}(PH(0, c)P) = \text{Rank}(PH(0, 0)P) \tag{5}
\]

for \( 0 < c < \eta \), and

\[
\text{Rank}(PH(0, \eta)P) < \text{Rank}(PH(0, 0)P) \tag{6}
\]

for \( c = \eta \) by Lemma 4.2.

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

\[
\text{Rank}(PH(0, c)P) = \text{Rank}(H(a_c, c)) = \text{Rank}(H(0, c)) - 1 \leq \text{Rank}(H(a, c)) \quad \tag{7}
\]

by Remarks 3.3 and 3.5.

1. Since \( H(0, \eta) \) satisfies condition (1) from Lemma 3.2, there exists \( a \in \mathbb{R} \) such that \( (a, \eta) \in U \). From (5), (6) and (7), for each \( (a, c) \in U \) with \( c \neq \eta \),

\[
\text{Rank}(H(0, \eta)) - 1 = \text{Rank}(H(a_{\eta}, \eta)) = \text{Rank}(PH(0, \eta)P) < \text{Rank}(PH(0, 0)P) = \text{Rank}(PH(0, c)P) \tag{8}
\]

\[
= \text{Rank}(H(a_c, c)) \leq \text{Rank}(H(a, c)).
\]

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

\[
\text{Rank}(H(0, \eta)) - 1 = \text{Rank}(H(a_{\eta}, \eta)) \leq \text{Rank}(H(a, \eta)) \tag{9}
\]

by (7). The assertion follows from (4), (8), and (9).
(2): Since the minimal representation of $G'$ is spherical, there exists $a' \in \mathbb{R}$ such that $H(a', 0)$ is positive semidefinite. Since $E'_0 \subset \mathfrak{j}^\perp$ by Remark 4.1, the null space of $H(a', 0)$ is also $E'_0$. By Theorem 3.8, there exists a positive number $\eta'$ such that $0 < \eta' < \eta$ and $H(a', \eta')$ is positive semidefinite. For each $(a, c) \in U$, it follows from (5) and (7) that

$$\text{Rank}(H(a_\eta', \eta')) = \text{Rank}(PH(0, \eta')P) = \text{Rank}(PH(0, 0)P)$$

$$= \text{Rank}(PH(0, c)P) \leq \text{Rank}(H(a, c)).$$

(10)

It follows from Lemma 2.4 and Remark 3.3 that

$$\text{Rank}(PH(0, 0)P) = \text{Rank}(H(0, 0)) - 1. \quad (11)$$

The assertion follows from (4), (10), and (11). \qed

### 5 Algorithm to Find the Largest 3-Codes

In this section, we construct an algorithm using only rational arithmetic to classify the largest 3-codes in $\Omega_1(d)$ 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 $\gamma$ 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 $\gamma$ is represented by a pair $(f_\gamma, I)$, where $f_\gamma$ is the minimal polynomial of $\gamma$ over the field of rationals, and $I$ is an isolating interval $[a, b]$ for $f_\gamma$ and $\gamma$. If $f$ is the minimal polynomial of $\gamma$, then $\gamma$ 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 5.1** [12] There is an algorithm (using only rational arithmetic) which takes as input an algebraic number $\gamma$ and a polynomial $f$ with integer coefficients, and determines the sign of the number $f(\gamma)$.

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

**Lemma 5.2** There is an algorithm (using only rational arithmetic) which takes as input a real algebraic number $\gamma$ and a symmetric matrix $M(t)$ whose entries are in $\mathbb{Q}[t]$, and determines the number of the positive and negative eigenvalues of $M(\gamma)$. This determines whether $M(\gamma)$ is positive semidefinite.

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

$$P(t, x) = |M(t) - xI|. \quad \square$$
Let $P_i(t)$ be the coefficient of $x^i$ in $P(x) = P(t, x)$. By Lemma 5.1, 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 $P_i(\gamma)$.

Let $f$ be an irreducible polynomial over $\mathbb{Q}(\gamma)$ for an algebraic integer $\gamma$. Let $\eta$ be a zero of $f$. Using Sturm’s theorem, $\eta$ can be represented by $(f, I)$, where $I$ is an isolating interval for $f$ and $\eta$. Here the signs in Sturm’s sequence can be determined by Lemma 5.1.

**Lemma 5.3** There is an algorithm (using only rational arithmetic) which takes as input an algebraic number $\gamma$, a real number $\eta$ 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 $\eta$ 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 $f(a)$.

**Lemma 5.4** There is an algorithm (using only rational arithmetic), which takes as input a real algebraic number $\gamma$, a real number $\eta$ that is a root of an irreducible polynomial over $\mathbb{Q}(\gamma)$, and a symmetric matrix $M(t, c)$ whose entries are in $\mathbb{Q}[t, c]$, and determines the number of positive and negative eigenvalues of $M(\gamma, \eta)$. This determines whether $M(\gamma, \eta)$ is positive semidefinite.

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

$$P(t, c, x) = |M(t, c) - xI|.$$ 

Let $P_i(t, c)$ be the coefficient of $x^i$ in $P(x) = P(t, c, x)$. By Lemma 5.3, we can determine the sign of $P_i(\gamma, \eta)$. Using Descartes’ rule of signs, the number of positive and negative roots of $P(x) = P(\gamma, \eta, x)$ is determined by the list of the signs of $P_i(\gamma, \eta)$.

**Lemma 5.5** There is an algorithm (using only rational arithmetic) which takes as input an algebraic number $\gamma$ and a matrix $M(t)$ whose entries are in $\mathbb{Q}[t]$, and determines whether $M(\gamma)$ is the distance matrix of a spherical set.

**Proof** First we determine whether $M(\gamma)$ is dissimilar. Let $P(t, a, x)$ be the polynomial defined by

$$P(t, a, x) = | - M(t) + aJ - xI|$$

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 condition that the coefficient of $a^j$ is not divisible by the minimal polynomial $f_\gamma$ of $\gamma$. If the coefficient of $a^j$ is divisible by $f_\gamma$ for each $j$, then we set...
Let \( x \) for an indeterminate set. Indeed, there is an algorithm that gives the factorization of an integral polynomial into irreducible polynomials over \( \mathbb{Q}(\gamma) \) [27]. The rank of \( PH(0)P \) is determined by Lemma 5.2. The value \( \eta \) 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 \( P_i(0) \).

Lemma 5.7 There is an algorithm (using only rational arithmetic) which takes as input a simple graph \( G \), and determines the type of \( G \).

Proof Let \( A \) be the adjacency matrix of \( G \). Let \( \lambda_i \) be the \( i \)-th smallest eigenvalue of \( A \), and \( m_i \) the multiplicity of \( \lambda_i \). Indeed, there is an algorithm that gives the factorization of an integral polynomial into irreducible polynomials over \( \mathbb{Q} \), see [28]. Let \( M(t) \) be the matrix defined by \( M(t) = -(t+1)A - t\overline{A} \) for an indeterminate \( t \). By Lemma 5.2, we can determine \( \text{Rank}(M(\lambda_i)) \) and \( \text{Rank}(PM(\lambda_i)P) \). By Lemma 2.4, Remark 3.3, and Theorems 2.2, 2.3, we can determine the type of \( G \) as follows: \( G \) is Type (1) if and only if \( \text{Rank}(PM(\lambda_1)P) = n - m_1 - 1 \), and \( M(\lambda_1) \) is the distance matrix of a spherical set. \( G \) is Type (2) if and only if \( m_1 > 1 \), \( \text{Rank}(PM(\lambda_1)P) = n - m_1 \), and \( M(\lambda_1) \) is the distance matrix of a spherical set. \( G \) is Type (3) if and only if \( m_1 = 1 \), \( \lambda_2 < -1 \), \( M(\lambda_2) \) is not the distance matrix of a spherical set, \( PM(\lambda_2)P \) is positive semidefinite, and \( \text{Rank}(PM(\lambda_2)P) = n - m_2 - 2 \). \( G \) is Type (4) if and only if \( m_1 = 1 \), \( \lambda_2 < -1 \), \( M(\lambda_2) \) is the distance matrix of a spherical set, and \( \text{Rank}(PM(\lambda_2)P) = n - m_2 - 1 \). If \( G \) is not of Type (i) for each \( i \) \( \in \{1, \ldots , 4\} \), then \( G \) is Type (5).

Lemma 5.8 Let \( G \) be an oriented graph with adjacency matrix \( A \). Let \( G' \) be either the simple graph with the adjacency matrix \( B = A + A^T \) or its complement. Suppose that \( G' \) is of Type (1), (2), or (4). If the null space of the minimal representation \( eB + \overline{B} \) is contained in that of \( A - A^T \), then there is an algorithm (using only rational arithmetic) which determines \( \text{Rep}(G) \).

\[ Q_i(t) = 0. \] By Lemma 5.1, we can determine the sign of \( Q_i(\gamma) \). For a sufficiently large \( a \), we can determine the sign of \( P_i(\gamma, a) \) as follows: \( P_i(\gamma, a) = 0 \) 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 negative roots of \( P(x) = P(\gamma, a, x) \) for a sufficiently large \( a \) is determined by the list of the signs of \( P_i(\gamma, a) \). By Lemma 2.5, \( m = 0 \) if and only if \( M \) is the distance matrix of a spherical set. \( \Box \)
Proof By Lemma 5.6, we can determine \( \eta \) such that \( -P(\xi B + \overline{B})P + \eta \sqrt{-1}P(A - A^T)P \) is a positive semidefinite matrix of rank less than \( \text{Rep}(G') \). Note that \( \text{Rep}(G') \) is determined by Lemma 5.7. If there exists a positive number \( a \) such that \( -(\xi B + \overline{B}) + \eta \sqrt{-1}(A - A^T) + aJ \) is positive semidefinite, then \( \text{Rep}(G) \) is the rank of \( -P(\xi B + \overline{B})P + \eta \sqrt{-1}P(A - A^T)P \), else \( \text{Rep}(G) = \text{Rep}(G') \) by Theorem 4.3. The existence of such number \( a \) can be checked by a similar manner to Lemma 5.5. Here the signs of coefficients are checked by Lemma 5.3.

Here 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 \( \gamma \). 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 2.3. The distance \( \gamma \) may be less than 1, and \( \gamma = (\lambda + 1)/\lambda \) holds, where \( \lambda \) is the smallest or second smallest eigenvalue of \( G \) by Theorem 2.2. First we produce \( L_0(\gamma) \) for any possible \( \gamma \) by applying Lemma 5.7 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 \( B \) be the adjacency matrix of \( G' \), and \( \overline{B} \) the adjacency matrix of the complement. Let \( M(\lambda) \) be the matrix \((\lambda + 1)B + \lambda\overline{B} \), where \( \lambda = 1/(\gamma - 1) \). Let \( \mathcal{E}_0 \) be the null space of \( M(\lambda) \). Let \( K(G') \) be the set of all oriented graphs \( G \) such that \( \mathcal{E}_0' \subseteq \mathcal{E}_0 \), \( A + A^T = B \) or \( \overline{B} \), and \( \text{Rep}(G) \leq d \), where \( A \) is the adjacency matrix of \( G \), and \( \mathcal{E}_0 \) is the null space of \( A - A^T \). Here, \( \text{Rep}(G) \) is determined by Lemma 5.8. Note that \( \mathcal{E}_0' \subseteq \mathcal{E}_0 \) if and only if the row space of \( A - A^T \) is contained in the row space of \( M(\lambda) \). Moreover, when \( \text{Rank}(M(\lambda)) = 2d \), we need \( \text{Rank}(A - A^T) = 2d \) in order to have \( \text{Rep}(G) = d \) by the proof of Theorem 3.7. These conditions can eliminate a large number of choices for \( A \). We can make the list of \( A \) and give \( \text{Rep}(G) \) for each \( A \). 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 for augmenting graph \( G' \in L(n, \gamma) \) by an \((n + 1)\)-th vertex are examined. There are \( 2^n \) possibilities for a newly added \((n + 1)\)-th row of \( B \). Its entries are in \( \{0, 1\} \). We may think of these \( 2^n \) sequences as leaves of a binary tree of depth \( n \). At a depth of at least \( 2d + 2 \), the search is effectively pruned by checking various sub-matrices of size \( 2d + 2 \) against the list \( L(2d + 2, \gamma) \). Let \( \tilde{B} \) be a new matrix obtained from \( B \) by adding a new column and a new row, and \( \tilde{G} \) the simple graph with the adjacency matrix \( \tilde{B} \). We check whether \( \tilde{G} \) already appears in \( L(n + 1, \gamma) \). If not, we then 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 \( \text{Rep}(\tilde{G}') \leq 2d \) if and only if all graphs \( \tilde{G}'_1, \ldots, \tilde{G}'_{2d+2}, G' \) appear 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 \( L(n, \gamma) \).
Table 1  Largest complex 3-codes in \( \Omega(d) \)

| \( d \) | 1 | 2 | 3 |
|---|---|---|---|
| \(|X|\) | 4 | 8 | 9 |
| \# | 1 | 1 | 50 |

The smallest number \( n \) such that \( L(n + 1, \gamma) \) is empty for any \( \gamma \) is the size of the 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. For \( d \geq 4 \), classification is not possible on a normal computer. For \( d = 1, 2 \), the largest complex 3-codes are tight, and they are considered in Sect. 6. For \( d = 3 \), one of the largest 3-codes is the union of three equilateral triangles in \( \mathbb{C} \), which are orthogonal to one another. For the other largest 3-codes \( X, \phi \left( X \cup e^{2 \pi \sqrt{-1}/3} X \cup e^{4 \pi \sqrt{-1}/3} X \right) \) is the unique largest 2-distance set in \( \mathbb{R}^6 \) [7,25], which is the minimal representation of the Schlafli 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 code, namely \( S \)-codes. A tight \( S \)-code with degree \( |S| - 1 \) 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 \( S \) of \( \mathbb{N}^2 \) is a lower set if the following condition is satisfied: if \( (i, j) \in \mathbb{N}^2 \) is in \( S \), 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 \( S \)-code if there exists a polynomial \( F(\alpha) = \sum_{(k,l) \in S} a_{k,l} x^k \bar{x}^l \) with real coefficients such that \( F(\alpha) = 0 \) for any \( \alpha \in D(X) \) and \( F(1) > 0 \).

We denote by \( \text{Hom}_d(k, l) \) 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 \( \text{Hom}_d(k, l) \), and the irreducible decomposition is

\[
\text{Hom}_d(k, l) = \bigoplus_{m=0}^{\min(k,l)} \text{Harm}_d(k-m, l-m),
\]

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

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

\[
\langle f, g \rangle := \int_{\Omega(d)} \overline{f(z)} g(z) \, dz.
\]
Here, $dz$ is the unique invariant Haar measure on $\Omega(d)$, normalized so that $\int_{\Omega(d)} dz = 1$. With respect to this inner product, $\text{Harm}_d(k, l)$ is orthogonal to $\text{Harm}_d(k', l')$ whenever $(k, l) \neq (k', l')$. For each $(k, l) \in \mathbb{N}^2$, we fix an orthonormal basis $\{e_1, \ldots, e_{m_{k,l}^d}\}$ for the space $\text{Harm}_d(k, l)$. For a finite set $X$ in $\Omega(d)$, we define the characteristic matrix $H_{k,l}$ with rows indexed by $X$ and columns indexed by $\{1, 2, \ldots, m_{k,l}^d\}$ as

$$(H_{k,l})_{x,i} = e_i(x)$$

for $x \in X$ and $i \in \{1, 2, \ldots, m_{k,l}^d\}$.

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

$$g_{k,l}^d(x) := \frac{m_{k,l}^d(d-2)!k!l!}{(d+k-2)!(d+l-2)!} \sum_{r=0}^{\min(k,l)} (-1)^r \frac{(d+k+l-r-2)!}{r!(k-r)!(l-r)!} x^{k-r} \bar{x}^{l-r},$$

where

$$m_{k,l}^d = \dim(\text{Harm}_d(k, l)) = \binom{d+k-1}{d-1} \binom{d+l-1}{d-1} - \binom{d+k-2}{d-1} \binom{d+l-2}{d-1}.$$  \hfill (12)

The Jacobi polynomials we used are

$$g_{0,0}^d(x) = 1,$$
$$g_{1,0}^d(x) = dx,$$
$$g_{0,1}^d(x) = d\bar{x},$$
$$g_{1,1}^d(x) = (d+1)(d\bar{x} - 1).$$

Recursively, the Jacobi polynomials satisfy

$$x g_{k,l}^d(x) = a_{k,l} g_{k+1,l}^d(x) + b_{k,l} g_{k,l-1}^d(x),$$  \hfill (13)

where $a_{k,l} = (k+1)/(d+k+l)$, $b_{k,l} = (d+l-2)/(d+k+l-2)$ and set $g_{k,l}^d(x) = 0$ 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 6.1** Let $\{e_1, \ldots, e_{m_{k,l}^d}\}$ be an orthonormal basis for the space $\text{Harm}_d(k, l)$. Then, for any $a, b \in \Omega(d)$,

$$\sum_{i=1}^{m_{k,l}^d} e_i(a) e_i(b) = g_{k,l}^d(a^* b).$$

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An upper bound on the size of an $S$-code is given as follows:

**Theorem 6.2** [23, Thm. 4.2(ii)] For $d \geq 2$, let $X$ be an $S$-code in $\Omega(d)$. Then $|X| \leq \sum_{(k,l) \in S} \dim(\mathrm{Harm}(k, l))$ holds.

An $S$-code is *tight* if equality holds in Theorem 6.2. Tight codes are related to complex spherical designs. For a finite lower set $T$, a finite subset $X$ of $\Omega(d)$ is a *complex spherical* $T$-design if, for every polynomial $f \in \mathrm{Hom}(k, l)$ such that $(k, l)$ is in $T$,

$$
\frac{1}{|X|} \sum_{z \in X} f(z) = \int_{\Omega(d)} f(z) \, dz,
$$

(14)

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

**Theorem 6.3** [23, Thm. 5.4] Let $X$ be a finite set in $\Omega(d)$ and let $S$ be a lower set. The following are then equivalent:

1. $X$ is a tight $S$-code.
2. $X$ is a tight $S \ast S$-design.
3. $X$ is an $S$-code and an $S \ast S$-design.

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

Let $X$ have an angle set $D(X) = \{\alpha_1, \ldots, \alpha_s\}$, and set $\alpha_0 = 1$. For $0 \leq i \leq s$, define the binary relation $R_i$ as the set of pairs $(x, y) \in X \times X$ such that $x^* y = \alpha_i$.

The following is a key theorem for characterizing tight 3-codes.

**Theorem 6.4** [23, Thm. 6.1] Let $X$ be a tight $S$-design with degree $s = |S| - 1$ for a lower set $S$. Then $X$ with binary relations defined from angles is a commutative association scheme. Moreover, the primitive idempotents are $\frac{1}{|X|} H_{k,l} H^*_{k,l}$, $(k, l) \in S$.

**Remark 6.5** If $X$ is a finite set in $\Omega(d)$, then the Gram matrix $G = (x^* y)_{x, y \in X}$ is $
\frac{1}{d} H_{0,1} 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 $i \in \{0, 1, \ldots, s\}$. The adjacency matrix $A_i$ of relation $R_i$ is defined as the $(0, 1)$-matrix with rows and columns indexed by $X$ such that $(A_i)_{x,y} = 1$ if $(x, y) \in R_i$ and $(A_i)_{x,y} = 0$ 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. $A_0$ is the identity matrix.
2. $\sum_{i=0}^s A_i = J$, where $J$ is the all-ones matrix.
3. For any $i \in \{0, 1, \ldots, s\}$, there exists $i' \in \{0, 1, \ldots, s\}$ such that $A_i^T = A_{i'}$.
4. For any $i, j, k \in \{0, 1, \ldots, s\}$, there exists $p_{i,j}^k$ such that $A_i A_j = \sum_{k=0}^s p_{i,j}^k A_k$.
5. $A_i A_j = A_j A_i$ for any $i, j$. Springer
The algebra $\mathcal{A}$ generated by all adjacency matrices $A_0, A_1, \ldots, A_s$ 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 $\{E_0, E_1, \ldots, E_s\}$ [3, Thm. 3.1]. Since $\{E_0^T, E_1^T, \ldots, E_s^T\}$ also forms the set of primitive idempotents, we define $\hat{i}$ by the index such that $E_{\hat{i}} = E_i^T$ 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** $q^k_{i,j}$, for $E_0, E_1, \ldots, E_s$ under the entrywise product:

$$|X|E_i \circ |X|E_j = |X| \sum_{k=0}^s q^k_{i,j} E_k.$$  

By the commutativity of the entrywise product, $q^k_{i,j} = q^k_{j,i}$ holds for any $i, j$. We need the following fundamental properties for the Krein parameters in the proof of Theorem 6.10.

**Lemma 6.6** Let $(X, \{R_i\}_{i=0}^s)$ be a commutative association scheme of class $s$, and let $q^k_{i,j}$ be its Krein parameters. Then the following hold for any $i, j, k, l$:

1. $q^k_{i,j} \geq 0$.
2. $q^0_{i,0} = \delta_{i,k}$.
3. $q^s_{i,j} = m_i \delta_{i,j}$.
4. $\sum_{j=0}^s q^k_{i,j} = m_i$.
5. $m_k q^k_{i,j} = m_j q^j_{i,k}$.
6. $\sum_{\alpha=0}^s q^\alpha_{i,j} q^l_{k,\alpha} = \sum_{\beta=0}^s q^\beta_{k,i} q^l_{\beta,j}$.

**Proof** See [3, Prop. 3.7, Thm. 3.8].

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

Both sets of matrices $\{A_0, A_1, \ldots, A_s\}$ and $\{E_0, E_1, \ldots, E_s\}$ are bases for the Bose–Mesner algebra. Therefore, there exists a change in basis matrices $P$ and $Q$ defined as follows:

$$A_i = \sum_{j=0}^s P_{ji} E_j, \quad E_j = \frac{1}{|X|} \sum_{i=0}^s Q_{ij} A_i.$$  

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

The Krein matrices $B^*_i$ and the second eigenmatrix $Q$ are related as follows: The proof is essentially the same as that of [3, Thm. 4.1]. A vector $v$ is **standard** if the first entry of $v$ is 1.
Lemma 6.7 Let \( (X, \{R_i\}_{i=0}^s) \) be a commutative association scheme with the Krein matrices \( B_i^\ast \) and the second eigenmatrix \( Q \). Let \( v_i = (Q_{i0}, Q_{i1}, \ldots, Q_{is}) \) be the \( i \)-th row of \( Q \) for \( i \in \{0, 1, \ldots, s\} \). Then \( v_i^T \) is characterized as the unique standardized common right eigenvector \( v^T \) of the Krein matrices \( B_i^\ast \) such that \( B_i^\ast v^T = Q_{ij} v^T \).

**Proof** We consider the left multiplication with respect to the entrywise product \( \circ \) as linear transformations and express them in matrix form with respect to \( \{E_0, E_1, \ldots, E_s\} \). We then have an algebra homomorphism \( \varphi \) from the Bose–Mesner algebra to \( \text{Mat}_{s+1}(\mathbb{C}) \) defined by \( \varphi(E_i) = (B_i^\ast)^T \). The rest of the proof is obtained by replacing the roles \( A_i, \mathbf{P} \) with \( E_i, Q \), respectively, in the proof of [3, Thm. 41(ii)]. \( \square \)

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

**Example 6.8** 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 [9]:

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

where \( \mu \) is any power of 2. The primitive idempotent \( E_1 \) then 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 \( D(X) = \{\alpha, \alpha, \beta\} \), where \( \alpha \) is an imaginary number and \( \beta \) is a real number. Note that \( \varphi(X) \) is a real \( s \)-code with \( s = 1 \) or 2. When \( d = 1 \), \( |X| = |\varphi(X)| \leq 5 \) with equality if and only if \( \varphi(X) \) is the regular 5-gon [7]. In this case, \( X \) has the 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 \( S \)-code, where \( S = \{(0, 0), (1, 0), (0, 1), (1, 1)\} \). By Theorem 6.2 with (12), we have the following upper bound for 3-codes:

\[ \square \]
Theorem 6.9  Let $X$ be a 3-code in $\Omega(d)$. Then

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

Note that the example for $d = 1$ coincides with the case of $\mu = 1$ in Example 6.8. However, a tight 3-code is rare, shown in the following theorem.

Theorem 6.10  Let $X$ be a 3-code in $\Omega(d)$ attaining equality in Theorem 6.9. 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 $\beta$ is a real number, $\beta = -1$. Then $\alpha = \sqrt{-1}$ as desired.

Let $d$ be an integer that is at least 2. Since $X$ is a tight $S$-code, $X$ is an $S \ast S$-design by Theorem 6.3. 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 6.4. Then the Gram matrix of $X$ is a scalar multiple of some primitive idempotent of the association scheme, say $E_1$. We arrange the ordering of the primitive idempotents so that $E_2 = E_1^T$ holds and $E_3$ is a real matrix. Then $\hat{1} = 2, \hat{2} = 1, \hat{3} = 3$ hold.

We will determine the Krein matrix $B_1^*$ and the second eigenmatrix $Q$. We use Lemma 6.6 (2),(3) to obtain $q_{1,0}^0 = q_{1,0}^2 = q_{1,0}^3 = q_{1,1}^0 = q_{1,1}^3 = 0, q_{1,0}^1 = 1$, and $q_{1,2}^0 = d$. By Theorem 6.4, we may set

$$E_1 = \frac{1}{|X|} H_{1,0} H_{1,0}^*,
E_2 = \frac{1}{|X|} H_{0,1} H_{0,1}^*,
E_3 = \frac{1}{|X|} H_{1,1} H_{1,1}^*.$$ 

By the recurrence (13), we have that $E_2 = \frac{1}{|X|} g_{0,1} \circ (\frac{|X|}{d} E_1)$ and $E_3 = \frac{1}{|X|} g_{1,1} \circ (\frac{|X|}{d} E_1)$, where $f \circ (M)$ denotes the matrix obtained by applying a function $f$ to each entry of a matrix $M$. 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 $q_{1,2}^1 = q_{1,2}^2 = q_{1,2}^3 = 0$ and $q_{1,1}^3 = \frac{d}{d+1}$ holds. Since $X$ is an $S \ast S$-design and $S \ast S$ contains $(2, 1), q_{1,1}^1 = 0$ holds by [23, Cor. 9.3(ii)]. By Lemma 6.6 (4), we have

$$q_{1,1}^1 + q_{1,1}^3 = d, \quad (15)$$
$$q_{1,1}^1 + q_{1,1}^3 = \frac{d^2}{d+1}. \quad (16)$$
We have $m_1 = \dim(\text{Harm}(1, 0)) = d$ and $m_3 = \dim(\text{Harm}(1, 1)) = d^2 - 1$ by (12). Substituting the values $m_1, m_3$ into the equation in Lemma 6.6 (5) for $(i, j, k) = (1, 1, 3)$, we have

\[
(d^2 - 1)q^3_{1,1} = dq^2_{1,3}.
\]

Using the equation in Lemma 6.6 (6) for $(i, j, k, l) = (1, 1, 2, 1)$, we have

\[
(q^2_{1,1})^2 + \frac{d^2 - 1}{d} q^3_{1,1}q^2_{1,3} = \frac{2d^2}{d + 1}.
\]

We solve (15)–(18) to obtain

\[
(q^2_{1,1}, q^3_{1,1}, q^2_{1,3}, q^3_{1,3}) = \begin{cases}
\left( \frac{d(d-(d-1)\sqrt{d+2})}{d^2+d-1}, \frac{d^2(d+1+\sqrt{d+2})}{(d+1)(d^2+d-1)}, \frac{d(d-1)(d+1+\sqrt{d+2})}{(d+1)(d^2+d-1)}, \frac{d(d^2-2-\sqrt{d+2})}{(d+1)(d^2+d-1)} \right),
\end{cases}
\]

First we consider the former case in (19). Since the Krein number $q^2_{1,1}$ is nonnegative by Lemma 6.6 (1), we must have $d = 2$. In this case the second eigenmatrix $Q$ is given by Lemma 6.7 as

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

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 6.7 as

\[
Q = \begin{pmatrix}
1 & t^2 - 2 & t^2 - 2 & (t^2 - 3)(t^2 - 1) \\
1 & \frac{t^2-2}{t+1} & \frac{t^2-2}{t+1} & \frac{(t+1)(t^2-3)}{t^2+7} \\
1 & (t^2 t + 1 + t \sqrt{-3 r^2 - 2 r + 5}) & (t^2 t + 1 + t \sqrt{-3 r^2 - 2 r + 5}) & -6 r t + 3 r^2 + 2 r^3 - t \sqrt{-3 r^2 - 2 r + 5} \\
1 & -6 r t + 3 r^2 + 2 r^3 - t \sqrt{-3 r^2 - 2 r + 5} & -6 r t + 3 r^2 + 2 r^3 - t \sqrt{-3 r^2 - 2 r + 5} & 4(t^2+2)(t^2+1) \\
\end{pmatrix}.
\]

The valency corresponding to the second row of the second eigenmatrix is then determined as $k_1 = (t + 1)^3(t^2 - 3)/(3t + 5)$ by $P = \frac{1}{|X|} Q^{-1}$. By substituting $t = \sqrt{d + 2}$, we find that the valency $k_1$ is equal to $(d - 1)(3d^2 + 6d + 5 + 4(d - 1) \sqrt{d + 2})/(9d - 7)$, which implies that $t = \sqrt{d + 2}$ must be an integer. The partial fraction decomposition $243k_1 = 81r^4 + 108r^3 - 180r^2 - 348t - 149 + 16/(3r + 5)$ shows that $3t + 5$ divides $16$. Since $t$ is positive, we have $t = 1$ and thus $d = -1$. This is contradictory to the fact that $d$ is positive. \qed
For $d = 1, 2$, the tight 3-code is unique, which is proved in Sect. 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 6.11** For $S = \{(0, 0), (1, 0), (0, 1), (1, 1)\}$, the tight $S$-codes with degree 4 were given in [23, Exam. 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] for more detail.

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