# STRENGTHENED SEMIDEFINITE PROGRAMMING BOUNDS FOR CODES 

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#### Abstract

We give a hierarchy of semidefinite upper bounds for the maximum size $A(n, d)$ of a binary code of word length $n$ and minimum distance at least $d$. At any fixed stage in the hierarchy, the bound can be computed (to an arbitrary precision) in time polynomial in $n$; this is based on a result of de Klerk, Pasechnik and Schrijver [2] about the regular *-representation for matrix *-algebras. The Delsarte bound for $A(n, d)$ is the first bound in the hierarchy, and the new bound of Schrijver [13] is located between the first and second bounds in the hierarchy. While computing the second bound involves a semidefinite program with $O\left(n^{7}\right)$ variables and thus seems out of reach for interesting values of $n$, Schrijver's bound can be computed via a semidefinite program of size $O\left(n^{3}\right)$, a result which uses the explicit block-diagonalization of the Terwilliger algebra. We propose two strengthenings of Schrijver's bound with the same computational complexity.


## 1. Introduction

We consider the problem of computing the parameter $A(n, d)$, defined as the maximum size of a binary code of word length $n$ and minimum distance at least $d$. With $\mathcal{P}$ denoting the collection of all subsets of $\{1, \ldots, n\}$, we can identify code words in $\{0,1\}^{n}$ with their supports; so a code $C$ is a subset of $\mathcal{P}$ and the Hamming distance of $I, J \in \mathcal{P}$ is equal to $|I \Delta J|$. The minimum distance of a code $C$ is the minimum Hamming distance of distinct elements of $C$. If we define the graph $\mathcal{G}(n, d)$ with node set $\mathcal{P}$, two nodes $I, J \in \mathcal{P}$ being adjacent if $|I \Delta J| \in\{1, \ldots, d-1\}$, then a code with minimum distance $d$ corresponds to a stable set in the graph $\mathcal{G}(n, d)$. Therefore, the parameter $A(n, d)$ is equal to the stability number of the graph $\mathcal{G}(n, d)$, i.e., the maximum cardinality of a stable set in $\mathcal{G}(n, d)$.

Schrijver [13] introduced recently an upper bound for $A(n, d)$ which refines the classical bound of Delsarte [3]. While Delsarte bound is based on diagonalizing the (commutative) Bose-Mesner algebra of the Hamming scheme and can be computed via linear programming, Schrijver's bound is based on block-diagonalizing the (non-commutative) Terwilliger algebra of the Hamming scheme and can be computed via semidefinite programming. In both cases the bounds can be formulated as the optimum of a (linear or semidefinite) program of size polynomial in $n$ (size $O(n)$ for Delsarte bound and size $O\left(n^{3}\right)$ for Schrijver's bound).

Finding tight upper bounds for the stability number $\alpha(\mathcal{G})$ of a graph $\mathcal{G}=(\mathcal{V}, \mathcal{E})$ has been the subject of extensive research. Lovász [9] introduced the theta number $\vartheta(\mathcal{G})$,

[^0]which can be computed, e.g., via the semidefinite program:
\[

$$
\begin{array}{ll}
\vartheta(\mathcal{G}):=\max \sum_{i \in \mathcal{V}} X_{i i} \text { s.t. } & X=\left(X_{i j}\right)_{i, j \in \mathcal{V} \cup\{0\}} \succeq 0, X_{00}=1  \tag{1}\\
& X_{0 i}=X_{i i}(i \in \mathcal{V}), X_{i j}=0(i j \in \mathcal{E})
\end{array}
$$
\]

The theta number can be computed (with arbitrary precision) in time polynomial in the number of nodes of the graph. Moreover, $\vartheta(\mathcal{G})=\alpha(\mathcal{G})$ when $\mathcal{G}$ is a perfect graph (see [5]). Schrijver [12] introduced the strenghtening $\vartheta^{\prime}(\mathcal{G})$ of $\vartheta(\mathcal{G})$ obtained by adding the nonnegativity constraint $X \geq 0$ to the program (1) and proved that $\vartheta^{\prime}(\mathcal{G}(n, d))$ coincides with Delsarte bound.

Various methods have been proposed in the litterature for constructing tighter semidefinite upper bounds for the stability number of a graph, in particular, by Lovász and Schrijver [10] and more recently by Lasserre [6, 7]. In both cases a hierarchy of upper bounds for $\alpha(\mathcal{G})$ is obtained with the property that the bound reached at the $\alpha(\mathcal{G})$-th iteration coincides in fact with $\alpha(\mathcal{G})$. It turns out that Lasserre's hierarchy refines the hierarchy of Lovász and Schrijver (see [8]).

For $k \geq 1$, denote by $\ell^{(k)}(\mathcal{G})$ the bound in Lasserre's hierarchy at the $k$-th iteration; see Section 3.1 for the precise definition. It is known (and easy to see) that, for fixed $k$, one can compute (with arbitrary precision) the parameter $\ell^{(k)}(\mathcal{G})$ in time polynomial in the number of nodes of the graph $\mathcal{G}$. However, for the coding problem, the graph $\mathcal{G}(n, d)$ has $2^{n}$ nodes and such complexity is prohibitive for large $n$. A first contribution of this paper (see Section 3.2) is to show that, for fixed $k$, the bound $\ell^{(k)}(\mathcal{G}(n, d))$ can be computed (with arbitrary precision) in time polynomial in $n$. This result is based on a result of de Klerk, Pasechnik and Schrijver [2], recalled in Section 2.1, about reducing the size of invariant semidefinite programs using the regular $*$-representation for the algebra of invariant matrices under action of a group.

The first bound $\ell^{(1)}(\mathcal{G})$ in the hierarchy is equal to the theta number $\vartheta(\mathcal{G})$; its strengthening obtained by adding nonnegativity is equal to $\vartheta^{\prime}(\mathcal{G})$ which, for the graph $\mathcal{G}=\mathcal{G}(n, d)$, coincides with the bound of Delsarte for the parameter $A(n, d)$. It turns out that the bound of Schrijver [13] for $A(n, d)$ lies between $\ell_{+}^{(1)}(\mathcal{G})$ and $\ell_{+}^{(2)}(\mathcal{G})$, the strengthenings of $\ell^{(1)}(\mathcal{G})$ and $\ell^{(2)}(\mathcal{G})$ obtained by adding certain bounds on the variables. While Schrijver's bound can be computed via a semidefinite program of size $O\left(n^{3}\right)$ and thus computed in practice for reasonable values of $n$, a practical computation of $\ell_{+}^{(2)}(\mathcal{G}(n, d))$ seems out of reach for interesting values of $n$ since one would have to solve a semidefinite program with $O\left(n^{7}\right)$ variables.

In Section 3.3, we introduce two bounds $\ell_{+}(\mathcal{G}(n, d))$ and $\ell_{++}(\mathcal{G}(n, d))$ satisfying

$$
\ell_{+}^{(2)}(\mathcal{G}(n, d)) \leq \ell_{++}(\mathcal{G}(n, d)) \leq \ell_{+}(\mathcal{G}(n, d)) \leq \ell_{+}^{(1)}(\mathcal{G}(n, d))
$$

they are at least as good as Schrijver's bound, and their computation still relies on solving a semidefinite program of size $O\left(n^{3}\right)$. This complexity result follows from the fact that the new bounds, analogously to Schrijver's bound, require the positive semidefiniteness of certain matrices lying in the Terwilliger algebra (or a variation of it) whose dimension is $O\left(n^{3}\right)$ and for which the explicit block-diagonalization has been given by Schrijver [13].

Some notation. We group here some notation that will be used throughout the paper. We set $V:=\{1, \ldots, n\}$ and $\mathcal{P}:=\mathcal{P}(V)$ denotes the collection of all subsets of the set $V$. For a finite set $\mathcal{V}$ and an integer $k \geq 1$, we set $\mathcal{P}_{k}(\mathcal{V}):=\{I \subseteq \mathcal{V}| | I \mid \leq k\}$ and $\mathcal{P}_{=k}(\mathcal{V}):=\{I \subseteq \mathcal{V}| | I \mid=k\}$. We let $\operatorname{Sym}(\mathcal{V})$ denote the set of all permutations of the set $\mathcal{V}$ and we set $\operatorname{Sym}(n):=\operatorname{Sym}(\mathcal{V})$ when $|\mathcal{V}|=n$. The letter $\mathcal{G}$ will be used to denote a graph, with node set $\mathcal{V}$ and edge set $\mathcal{E}$, while the letter $G$ will be used to denote a group (e.g., of automorphisms of $\mathcal{G}$ ).

## 2. Algebraic Preliminaries

2.1. Preliminaries on invariant matrices. Let $G$ be a finite group acting on a finite set $\mathcal{X}$; that is, we have a homomorphism $h: G \rightarrow \operatorname{Sym}(\mathcal{X})$, where $\operatorname{Sym}(\mathcal{X})$ is the group of permutations of $\mathcal{X}$. For $\sigma \in G, h(\sigma)$ is a permutation of $\mathcal{X}$ and $M_{\sigma}$ is the associated $\mathcal{X} \times \mathcal{X}$ permutation matrix with

$$
\left(M_{\sigma}\right)_{x, y}= \begin{cases}1 & \text { if } h(\sigma)(x)=y \\ 0 & \text { otherwise }\end{cases}
$$

The set:

$$
\mathcal{A}:=\left\{\sum_{\sigma \in G} \lambda_{\sigma} M_{\sigma} \mid \lambda_{\sigma} \in \mathbb{R}(\sigma \in G)\right\}
$$

is a matrix *-algebra; that is, $\mathcal{A}$ is closed under addition, scalar and matrix multiplication, and conjugation.

Any $\sigma \in G$ acts on matrices indexed by the set $\mathcal{X}$. Namely, for a $\mathcal{X} \times \mathcal{X}$ matrix $N$ and $\sigma \in G$, set

$$
\sigma(N):=\left(N_{\sigma(x), \sigma(y)}\right)_{x, y \in \mathcal{X}}
$$

The matrix $N$ is said to be invariant under the action of $G$ if $\sigma(N)=N$ for all $\sigma \in G$. Then the commutant algebra $\mathcal{A}^{G}$ of the algebra $\mathcal{A}$, defined by

$$
\mathcal{A}^{G}:=\left\{N \in \mathbb{C}^{\mathcal{X} \times \mathcal{X}} \mid N M=M N \forall M \in \mathcal{A}\right\}
$$

consists precisely of the $\mathcal{X} \times \mathcal{X}$ matrices $N$ that are invariant under the action of $G ; \mathcal{A}^{G}$ is again a matrix $*$-algebra.

The orbit of $(x, y) \in \mathcal{X} \times \mathcal{X}$ under action of $G$ is the set $\{(\sigma(x), \sigma(y)) \mid \sigma \in G\}$. Let $\mathcal{O}_{1}, \ldots, \mathcal{O}_{N}$ denote the orbits of the set $\mathcal{X} \times \mathcal{X}$ under the action of the group $G$ and, for $i=1, \ldots, N$, let $\tilde{D}_{i}$ be the $\mathcal{X} \times \mathcal{X}$ matrix:

$$
\left(\tilde{D}_{i}\right)_{x, y}= \begin{cases}1 & \text { if }(x, y) \in \mathcal{O}_{i}  \tag{2}\\ 0 & \text { otherwise }\end{cases}
$$

Then, $\tilde{D}_{1}, \ldots, \tilde{D}_{N}$ form a basis of the commutant $\mathcal{A}^{G}$ (as vector space) and $\tilde{D}_{1}+\ldots+\tilde{D}_{N}=$ $J$ (the all-ones matrix). We normalize the $\tilde{D}_{i}$ to

$$
\begin{equation*}
D_{i}:=\frac{\tilde{D}_{i}}{\sqrt{\left\langle\tilde{D}_{i}, \tilde{D}_{i}\right\rangle}} \tag{3}
\end{equation*}
$$

for $i=1, \ldots, N$. (For two $N \times N$ matrices $\left.A, B,\langle A, B\rangle:=\operatorname{Tr}\left(A^{T} B\right)=\sum_{i, j=1}^{N} A_{i j} B_{i j}.\right)$ Then, $\left\langle D_{i}, D_{j}\right\rangle=1$ if $i=j$ and 0 otherwise. The multiplication parameters $\gamma_{i, j}^{k}$ are defined by

$$
\begin{equation*}
D_{i} D_{j}=\sum_{k=1}^{N} \gamma_{i, j}^{k} D_{k} \tag{4}
\end{equation*}
$$

for all $i, j=1, \ldots, N$. Define the $N \times N$ matrices $L_{1}, \ldots, L_{N}$ by

$$
\begin{equation*}
\left(L_{k}\right)_{i, j}:=\gamma_{k, j}^{i} \text { for } k, i, j=1, \ldots, N \tag{5}
\end{equation*}
$$

De Klerk, Pasechnik and Schrijver [2] show:
THEOREM 1. The mapping $D_{k} \mapsto L_{k}$ is a $*$-isomorphism, known as the regular $*$-representation of $\mathcal{A}^{G}$. In particular, given real scalars $x_{1}, \ldots, x_{N}$,

$$
\begin{equation*}
\sum_{i=1}^{N} x_{i} D_{i} \succeq 0 \Longleftrightarrow \sum_{i=1}^{N} x_{i} L_{i} \succeq 0 \tag{6}
\end{equation*}
$$

This result has important algorithmic applications, as it permits to give more compact formulations for invariant semidefinite programs. Consider a semidefinite program:

$$
\begin{equation*}
\min \langle C, Y\rangle \text { s.t. }\left\langle A_{\ell}, Y\right\rangle \leq b_{\ell}(\ell=1, \ldots, m), Y \succeq 0 \tag{7}
\end{equation*}
$$

in the $\mathcal{X} \times \mathcal{X}$ matrix variable $Y$. Assume that the program (7) is invariant under action of the group $G$; that is, $C$ is invariant under action of $G$ and, for every matrix $Y$ feasible for (7) and $\sigma \in G$, the matrix $\sigma(Y)$ is again feasible for $Y$. (This holds, e.g., if the class of constraints is invariant under action of $G$, i.e., if for each $\ell \in\{1, \ldots, m\}$ and $\sigma \in G$, there exists $\ell^{\prime} \in\{1, \ldots, m\}$ such that $\sigma\left(A_{\ell}\right)=A_{\ell^{\prime}}$ and $b_{\ell}=b_{\ell^{\prime}}$.) Then, if $Y$ is feasible for (7) then the matrix $Y_{0}:=\frac{1}{|G|} \sum_{\sigma \in G} \sigma(Y)$ too is feasible for (7), with the same objective value as $Y$. Therefore, in (7), one can assume without loss of generality that $Y$ is invariant under action of $G$; that is, $Y$ is of the form $Y=\sum_{i=1}^{N} x_{i} D_{i}$ with $x_{1}, \ldots, x_{N} \in \mathbb{R}$. Then the objective function reads $\langle C, Y\rangle=\sum_{i=1}^{N} c_{i} x_{i}$, after setting $C=\sum_{i=1}^{N} c_{i} D_{i}$, and the constraints in (7) become linear constraints in $x$. As a direct application of Theorem 1 , we find:

Corollary 2. Consider the program (7) in the $\mathcal{X} \times \mathcal{X}$ matrix variable $Y$. If (7) is invariant under the action of the group $G$, then it can be equivalently reformulated as

$$
\begin{equation*}
\min \sum_{i=1}^{N} c_{i} x_{i} \text { s.t. } a_{\ell}^{T} x \leq b_{\ell}(\ell=1, \ldots, m), \sum_{i=1}^{N} x_{i} L_{i} \succeq 0 \tag{8}
\end{equation*}
$$

The program (8) involves $N \times N$ matrices and $N$ variables. Here, $N$ is the dimension of the algebra $\mathcal{A}^{G}$ (the set of $\mathcal{X} \times \mathcal{X}$ invariant matrices under the action of the group $G$ ), typically much smaller than $|\mathcal{X}|$.

To use computationally this result, one needs to know explicitly the matrices $L_{1}, \ldots, L_{N}$, which involves computing the cardinality of the orbits of $\mathcal{X} \times \mathcal{X}$ and the multiplication parameters $\gamma_{i, j}^{k}$ in (4). De Klerk, Pasechnik and Schrijver [2] apply this technique for computing tighter bounds for the crossing number of a complete bipartite graph. We
apply it in Section 3.2 for reducing the size of the semidefinite programs permitting to compute the hierarchy of semidefinite bounds for the parameter $A(n, d)$.
Example 3. Let $\mathcal{X}:=\mathcal{P}$, the collection of all subsets of the set $V=\{1, \ldots, n\}$, and $G:=\operatorname{Sym}(V)$, the group of permutations of $V$. Each $\pi \in G$ induces a permutation of $\mathcal{X}$, again denoted by $\pi$, by letting $\pi(I):=\{\pi(i) \mid i \in I\}$ for $I \in \mathcal{P}$. Two pairs $(I, J),\left(I^{\prime}, J^{\prime}\right)$ $\left(I, J, I^{\prime}, J^{\prime} \in \mathcal{P}\right)$ lie in the same orbit [i.e., $I^{\prime}=\pi(I), J^{\prime}=\pi(J)$ for some $\left.\pi \in G\right]$ if and only if $|I|=\left|I^{\prime}\right|,|J|=\left|J^{\prime}\right|$ and $|I \cap J|=\left|I^{\prime} \cap J^{\prime}\right|$. Therefore, the commutant algebra $\mathcal{A}^{G}$ is generated by the matrices $M_{i, j}^{t}\left(i, j, t \in \mathbb{Z}_{+}\right)$, where

$$
\left(M_{i, j}^{t}\right)_{I, J}:= \begin{cases}1 & \text { if }|I|=i,|J|=j,|I \cap J|=t,  \tag{9}\\ 0 & \text { otherwise }\end{cases}
$$

for $I, J \in \mathcal{P} ; \mathcal{A}^{G}=: \mathcal{A}_{n}$ is known as the Terwilliger algebra of the Hamming scheme (Terwilliger [15]).

Example 4. Consider again the set $\mathcal{X}:=\mathcal{P}$, but now the group is $G:=\operatorname{Aut}(\mathcal{P})$, the automorphism group of $\mathcal{P}$. The group $G$ consists of the permutations $\sigma \in \operatorname{Sym}(\mathcal{P})$ preserving the symmetric difference, i.e., for which $|\sigma(I) \Delta \sigma(J)|=|I \Delta J|$ for all $I, J \in \mathcal{P}$. Thus,

$$
\begin{equation*}
G=\left\{\pi s_{A} \mid A \subseteq V, \pi \in \operatorname{Sym}(V)\right\} \tag{10}
\end{equation*}
$$

where, for a set $A \subseteq V, s_{A}$ is the permutation of $\mathcal{P}$ mapping any $I \in \mathcal{P}$ to $s_{A}(I):=A \Delta I$; we have $|G|=2^{n} n$ !. Two pairs $(I, J),\left(I^{\prime}, J^{\prime}\right)\left(I, J, I^{\prime}, J^{\prime} \in \mathcal{P}\right)$ lie in the same orbit [i.e., $I^{\prime}=\sigma(I), J^{\prime}=\sigma(J)$ for some $\left.\sigma \in G\right]$ if and only if $|I \Delta J|=\left|I^{\prime} \Delta J^{\prime}\right|$. Therefore, the algebra $\mathcal{A}^{G}$ is generated by the matrices $M_{k}(k=0,1, \ldots, n)$ where

$$
\left(M_{k}\right)_{I, J}:= \begin{cases}1 & \text { if }|I \Delta J|=k,  \tag{11}\\ 0 & \text { otherwise }\end{cases}
$$

for $I, J \in \mathcal{P} ; \mathcal{A}^{G}=: \mathcal{B}_{n}$ is known as the Bose Mesner algebra of the Hamming scheme. The Bose-Mesner algebra is a subalgebra of the Terwilliger algebra, as $M_{k}=\sum_{i, j=0}^{n} M_{i, j}^{(i+j-k) / 2}$ for $k=0,1, \ldots, n$.

In fact, it is known from invariant theory and $C *$-algebra theory that the algebra $\mathcal{A}^{G}$ can be block-diagonalized. Therefore, there exists a semidefinite program equivalent to the invariant program (7), where the matrix $Y$ is replaced by a block-diagonal matrix with possibly repeated blocks; see, e.g., Gaterman and Parrilo [4]. Such program is typically more compact than the program (8). However, finding explicitly the block-diagonalization is a nontrivial task in general. An advantage of the above mentioned reduction method, based on the regular $*$-representation, is that it involves the matrices $L_{i}$ which are explicitly defined in terms of the matrices $D_{i}$ generating the algebra. Nevertheless, Schrijver [13] was able to determine explicitly the block-diagonalization for the Terwilliger algebra; we recall this result in the next section as we will need it for the computation of our stronger bounds for the coding problem.
2.2. Block-diagonalization of the Terwilliger algebra. While the Bose-Mesner algebra $\mathcal{B}_{n}$ is a commutative algebra and thus can be diagonalized (see [3]), the Terwilliger algebra $\mathcal{A}_{n}$ is a non-commutative algebra. Its dimension is $\operatorname{dim} \mathcal{A}_{n}=\binom{n+3}{3}$, which is the number of triples $(i, j, t)$ for which $M_{i, j}^{t} \neq 0$. As $\mathcal{A}_{n}$ is a matrix $*$-algebra containing the
identity, it can be block-diagonalized, which means the following: There exists a unitary $\mathcal{P} \times \mathcal{P}$ complex matrix $U$ (i.e., $U^{*} U=I$ ) and positive integers $m$ and $p_{0}, q_{0}, \ldots, p_{m}, q_{m}$ such that the set $U^{*} \mathcal{A}_{n} U:=\left\{U^{*} M U \mid M \in \mathcal{A}_{n}\right\}$ is equal to the collection of block-diagonal matrices

$$
\left(\begin{array}{cccc}
C_{0} & 0 & \ldots & 0 \\
0 & C_{1} & \ldots & 0 \\
\vdots & \vdots & \ddots & 0 \\
0 & 0 & \ldots & C_{m}
\end{array}\right)
$$

where each $C_{k}(k=0,1, \ldots, m)$ is a block-diagonal matrix with $q_{k}$ identical blocks $B_{k}$ of order $p_{k}$ :

$$
C_{k}=\left(\begin{array}{cccc}
B_{k} & 0 & \ldots & 0 \\
0 & B_{k} & \ldots & 0 \\
\vdots & \vdots & \ddots & 0 \\
0 & 0 & \ldots & B_{k}
\end{array}\right)
$$

thus $2^{n}=\sum_{k=0}^{m} p_{k} q_{k}$ and $\sum_{k=0}^{m} p_{k}^{2}=\operatorname{dim} \mathcal{A}_{n}=\binom{n+3}{3}$. By deleting copies of identical blocks, it follows that $\mathcal{A}_{n}$ is isomorphic to the algebra

$$
\bigoplus_{k=0}^{m} \mathbb{C}^{p_{k} \times p_{k}}=\left\{\left.\left(\begin{array}{cccc}
B_{0} & 0 & \cdots & 0  \tag{12}\\
0 & B_{1} & \cdots & 0 \\
\vdots & \vdots & \ddots & 0 \\
0 & 0 & \cdots & B_{m}
\end{array}\right) \right\rvert\, B_{k} \in \mathbb{C}^{p_{k} \times p_{k}} \text { for } k=0,1, \ldots, m\right\}
$$

An important fact for our purpose is that this isomorphism preserves positive semidefiniteness. The existence of a unitary matrix $U$ with the above properties is standard $C *$-algebra theory (see, e.g., [14]). Schrijver [13] has constructed explicitly this matrix $U$ and the image of a matrix $M \in \mathcal{A}_{n}$ in the algebra (12). We recall some facts from [13] needed for our treatment; we refer to [13] for details and proofs.

It turns out that $U$ is real valued, $m=\left\lfloor\frac{n}{2}\right\rfloor$ and, for $k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$, the block $B_{k}$ has order $p_{k}=n-2 k+1$ and multiplicity $q_{k}=\binom{n}{k}-\binom{n}{k-1}$. In particular, the block $B_{0}$ has order $n+1$ and multilplicity 1 . We now describe explicitly the matrix $U$. For this, for $k=1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$, define

$$
\mathcal{L}_{k}:=\left\{b \in \mathbb{R}^{\mathcal{P}} \mid M_{k-1, k}^{k-1} b=0 \text { and } b_{I}=0 \text { if }|I| \neq k\right\} .
$$

Let $\mathcal{B}_{k}$ be a basis of $\mathcal{L}_{k}$. Then $\left|\mathcal{B}_{k}\right|=\binom{n}{k}-\binom{n}{k-1}$ and $\sum_{I \in \mathcal{P}} b_{I}=0$ for $b \in \mathcal{L}_{k}$. Set $\mathcal{B}_{0}:=\left\{b_{0}\right\}$ where $b_{0}:=(1,0, \ldots, 0)^{T} \in \mathbb{R}^{\mathcal{P}}$ (the nonzero entry being indexed by $\emptyset \in \mathcal{P}$ ) and define

$$
\mathcal{Q}:=\left\{(k, b, i) \left\lvert\, k \in\left\{0, \ldots,\left\lfloor\frac{n}{2}\right\rfloor\right\}\right., b \in \mathcal{B}_{k}, i \in\{k, k+1, \ldots, n-k\}\right\}
$$

Then $|\mathcal{Q}|=2^{n}=|\mathcal{P}|$. For $(k, i, b) \in \mathcal{Q}$, define the vector

$$
u_{k, i, b}:=\binom{n-2 k}{i-k}^{-\frac{1}{2}} M_{i, k}^{k} b \in \mathbb{R}^{\mathcal{P}}
$$

Finally define $U$ as the $\mathcal{P} \times \mathcal{Q}$ matrix whose columns are the vectors $u_{k, i, b}$ for $(k, i, b) \in \mathcal{Q}$. The following is shown in [13].

Proposition 5. [13] The matrix $U$ is orthogonal, i.e., $U^{T} U=I$. Moreover, for a matrix $M=\sum_{i, j, t=0}^{n} x_{i, j}^{t} M_{i, j}^{t} \in \mathcal{A}_{n}$ (with $x_{i, j}^{t} \in \mathbb{R}$ ), the matrix $U^{T} M U$ is a block-diagonal matrix determined by the partition of $\mathcal{Q}$ into the classes $\mathcal{Q}_{k, b}:=\{(k, i, b) \mid k \leq i \leq n-k\}$ (for $\left.k=0, \ldots,\left\lfloor\frac{n}{2}\right\rfloor, b \in \mathcal{B}_{k}\right)$. For a given integer $k=0, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$, the blocks corresponding to the classes $\mathcal{Q}_{k, b}\left(\right.$ for $\left.b \in \mathcal{B}_{k}\right)$ are all identical to the following matrix:

$$
\begin{equation*}
B_{k}(x):=\left(\sum_{t}\binom{n-2 k}{i-k}^{-\frac{1}{2}}\binom{n-2 k}{j-k}^{-\frac{1}{2}} \beta_{i, j, k}^{t} x_{i, j}^{t}\right)_{i, j=k}^{n-k} \tag{13}
\end{equation*}
$$

after setting

$$
\begin{equation*}
\beta_{i, j, k}^{t}:=\sum_{u=0}^{n}(-1)^{t-u}\binom{u}{t}\binom{n-2 k}{n-k-u}\binom{n-k-u}{i-u}\binom{n-k-u}{j-u} \tag{14}
\end{equation*}
$$

for $i, j, k, t \in\{0, \ldots, n\}$. As $\mathcal{A}_{n}$ is isomorphic to the algebra (12), we have:

$$
\begin{equation*}
\sum_{i, j, t=0}^{n} x_{i, j}^{t} M_{i, j}^{t} \succeq 0 \Longleftrightarrow B_{k}(x) \succeq 0 \quad \text { for } k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor . \tag{15}
\end{equation*}
$$

The above property (15) is the key tool used in [13] and in the present paper, which allows reducing semidefinite programs involving matrices in the Terwilliger algebra to semidefinite programs of size $O\left(n^{3}\right)$.

We will deal in this paper with matrices of the form

$$
\tilde{M}=\left(\begin{array}{ll}
d & c^{T}  \tag{16}\\
c & M
\end{array}\right), \quad \text { where } M=\sum_{i, j, t=0}^{n} x_{i, j}^{t} M_{i, j}^{t}, \quad d \in \mathbb{R}, c=\sum_{i=0}^{n} c_{i} \chi^{\mathcal{P}=i(V)}
$$

Recall that $\mathcal{P}_{=i}(V)=\{I \subseteq V| | I \mid=i\}$ and $\chi^{\mathcal{P}=i(V)} \in\{0,1\}^{\mathcal{P}}$ whose $I$-th entry is 1 if and only if $I \in \mathcal{P}_{=i}(V)$.
Lemma 6. The matrix $\tilde{M}$ from (16) is positive semidefinite if and only if $B_{k}(x) \succeq 0$ for $k=1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$, and

$$
\tilde{B}_{0}(x):=\left(\begin{array}{cc}
d & \tilde{c}^{T} \\
\tilde{c} & B_{0}(x)
\end{array}\right) \succeq 0, \text { where } \tilde{c}:=\left(c_{i}\binom{n}{i}^{\frac{1}{2}}\right)_{i=0}^{n}
$$

Proof. Setting

$$
\tilde{U}:=\left(\begin{array}{cc}
1 & 0 \\
0 & U^{T}
\end{array}\right)
$$

we have:

$$
\tilde{U}^{T} \tilde{M} \tilde{U}=\left(\begin{array}{cc}
d & c^{T} U \\
U^{T} c & U^{T} M U
\end{array}\right)
$$

It suffices now to verify that $\left(c^{T} U\right)_{k, i, b}=c^{T} u_{k, i, b}=0$ for $(k, i, b) \in \mathcal{Q}$ with $k \geq 1$, and that $\left(c^{T} U\right)_{0, i, b_{0}}=c_{i}\binom{n}{i}^{\frac{1}{2}}$ for $i=0, \ldots, n$. This is direct verification using the above definitions;
details are omitted. Hence, $\tilde{U}^{T} \tilde{M} \tilde{U}$ is block-diagonal, with blocks $\tilde{B}_{0}(x)$ (with multiplicity 1 ) and $B_{k}(x)$ (with multiplicity $q_{k}$ ) for $k=1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$. The lemma now follows.

## 3. SEmidefinite programming bounds for the stability number of a graph

3.1. Lasserre's construction. Let $\mathcal{G}=(\mathcal{V}, \mathcal{E})$ be a graph. A stable set in $\mathcal{G}$ is a set $S \subseteq \mathcal{V}$ containing no edge and the stability number $\alpha(\mathcal{G})$ of $\mathcal{G}$ is the maximum cardinality of a stable set in $\mathcal{G}$. Recall $\mathcal{P}_{k}(\mathcal{V})=\{I \subseteq \mathcal{V}| | I \mid \leq k\}$ for an integer $k$. Given a stable set $S$ in $\mathcal{G}$, define $x=\left(x_{I}\right)_{I \in \mathcal{P}_{k}(\mathcal{V})} \in\{0,1\}^{\mathcal{P}_{k}(\mathcal{V})}$ and $y=\left(y_{I}\right)_{I \in \mathcal{P}_{2 k}(\mathcal{V})} \in\{0,1\}^{\mathcal{P}_{2 k}(\mathcal{V})}$ with $x_{I}=1$ (resp., $y_{I}=1$ ) if and only if $I \subseteq S$, for $I \in \mathcal{P}_{k}(\mathcal{V})$ (resp., for $I \in \mathcal{P}_{2 k}(\mathcal{V})$ ). Then $y$ and the matrix $Y:=x x^{T}$ satisfy:

$$
\begin{gather*}
Y \succeq 0  \tag{17}\\
Y_{I, J}=y_{I \cup J} \quad\left(\text { for } I, J \in \mathcal{P}_{k}(\mathcal{V})\right)  \tag{18}\\
Y_{I, J}=y_{I \cup J}=0 \text { if } I \cup J \text { contains an edge }\left(\text { for } I, J \in \mathcal{P}_{k}(\mathcal{V})\right)  \tag{19}\\
Y_{\emptyset, \emptyset}=y_{\emptyset}=1  \tag{20}\\
\left.0 \leq y_{I} \leq y_{J} \text { if } J \subseteq I \text { (for } I, J \in \mathcal{P}_{2 k}(\mathcal{V})\right) \tag{21}
\end{gather*}
$$

We refer to (19) as the edge condition and to (18) as the moment condition. A matrix $Y$ satisfying (18) is known as a moment matrix and is denoted as $Y=M_{k}(y)$ (see $[6,7,8]$ ). Under the assumption (17), the edge condition (19) is, in fact, equivalent to $y_{i j}=0$ (for $i j \in \mathcal{E}$ ). (Here and below, we set $y_{i j}:=y_{\{i\},\{j\}}, y_{i}:=y_{\{i\}}$, etc.) Under (17), relation (21) holds for $I \in \mathcal{P}_{k}(\mathcal{V})$; indeed, the principal submatrix of $M_{k}(y)$ indexed by $\{I, J\}$ has the form $\left(\begin{array}{ll}y_{I} & y_{I} \\ y_{I} & y_{J}\end{array}\right)$, whose positive semidefiniteness implies $0 \leq y_{J} \leq y_{I}$. On the other hand, $M_{1}(y) \succeq 0$ implies $\left|y_{i j}\right| \leq \max \left(y_{i}, y_{j}\right)$; indeed the principal submatrix of $M_{1}(y)$ indexed by $\{\{i\},\{j\}\}$ has the form $\left(\begin{array}{cc}y_{i} & y_{i j} \\ y_{i j} & y_{j}\end{array}\right)$, whose positive semidefiniteness implies $y_{i j}^{2} \leq y_{i} y_{j} \leq \max \left(y_{i}^{2}, y_{j}^{2}\right)$. Similarly, $M_{2}(y) \succeq 0$ implies that $\left|y_{i j k}\right|$ is at most the largest two values among $y_{i j}, y_{i k}, y_{j k}$; indeed the principal submatrix of $M_{2}(y)$ indexed by $\{\{i, j\},\{i, k\},\{j, k\}\}$ has the form $\left(\begin{array}{lll}y_{i j} & y_{i j k} & y_{i j k} \\ y_{i j k} & y_{i k} & y_{i j k} \\ y_{i j k} & y_{i j k} & y_{j k}\end{array}\right)$, whose positive semidefiniteness implies $y_{i j k}^{2} \leq \min \left(y_{i j} y_{i k}, y_{i j} y_{j k}, y_{i k} y_{j k}\right) \leq y_{i k}^{2}, y_{j k}^{2}$ assuming, say, that $y_{i j} \leq y_{i k} \leq y_{j k}$.

Consider the semidefinite program:

$$
\begin{equation*}
\ell^{(k)}(\mathcal{G}):=\max \sum_{i \in \mathcal{V}} y_{i} \text { s.t. } M_{k}(y) \succeq 0, y_{\emptyset}=1, y_{i j}=0(i j \in \mathcal{E}) \tag{22}
\end{equation*}
$$

Then, $\alpha(\mathcal{G}) \leq \ell^{(k)}(\mathcal{G})$, with equality if $k \geq \alpha(\mathcal{G})([7,8])$. Define $\ell_{+}^{(k)}(\mathcal{G})$ as the parameter obtained by adding to (22) the constraints (21); thus,

$$
\alpha(\mathcal{G}) \leq \ell_{+}^{(k)}(\mathcal{G}) \leq \ell^{(k)}(\mathcal{G}) .
$$

For $k=1, \ell^{(1)}(\mathcal{G})=\vartheta(\mathcal{G})$, the Lovász' theta number, and the stronger bound obtained by adding nonnegativity to $(22)$ is $\vartheta^{\prime}(\mathcal{G})$, the strengthening of $\vartheta(\mathcal{G})$ introduced by McEliece, Rodemich and Rumsey [11] and Schrijver [12]. The bound $\ell^{(2)}(\mathcal{G})$ is at least as good as the parameter obtained by optimizing over $N_{+}(\mathrm{TH}(\mathcal{G}))$, the convex relaxation of the stable set polytope of $\mathcal{G}$ obtained by applying the Lovász-Schrijver $N_{+}$-operator to the theta body $\operatorname{TH}(\mathcal{G})([8] ;$ or see $(26))$. For $k=2$, the program (22) has size $O\left(|\mathcal{V}|^{4}\right)$. We now formulate a bound $\ell(\mathcal{G})$, which is weaker than $\ell^{(2)}(\mathcal{G})$, but still at least as good as the bound obtained from $N_{+}(\mathrm{TH}(\mathcal{G}))$, although its computation is more economical since it can be expressed via a semidefinite program of size $O\left(|\mathcal{V}|^{3}\right)$.

Namely, for each $r \in \mathcal{V}$, consider the principal submatrix $Y_{r}(y)$ of $M_{2}(y)$ indexed by the set $\mathcal{P}_{2}(\mathcal{V} ; r):=\mathcal{P}_{1}(\mathcal{V}) \cup\{\{r, i\} \mid i \in \mathcal{V}\}$; thus the matrices $Y_{r}(y)$ involve only variables $y_{I}$ for $I \in \mathcal{P}_{3}(\mathcal{V})$. Define

$$
\begin{equation*}
\ell(\mathcal{G}):=\max \sum_{i \in \mathcal{V}} y_{i} \text { s.t. } y_{\emptyset}=1, y_{i j}=0(i j \in \mathcal{E}), Y_{r}(y) \succeq 0(r \in \mathcal{V}) \tag{23}
\end{equation*}
$$

and $\ell_{+}(\mathcal{G})$ as the parameter obtained by adding to (23) the constraints: $0 \leq y_{i j k} \leq y_{i j}$ for distinct $i, j, k \in \mathcal{V}$ (coming from (21)). Obviously,

$$
\ell^{(2)}(\mathcal{G}) \leq \ell(\mathcal{G}) \leq \ell^{(1)}(\mathcal{G})
$$

analogously for the $\ell_{+}$parameters. We will see in Section 3.3 that, for the graph $\mathcal{G}=$ $\mathcal{G}(n, d)$, the matrices involved in (23) lie in (a variation of) the Terwilliger algebra, which allows reformulating the parameters $\ell(\mathcal{G}(n, d)), \ell_{+}(\mathcal{G}(n, d))$ via semidefinite programs of size $O\left(n^{3}\right)$.

From the moment condition (18), the matrix $Y_{r}(y)$ has the block structure:

$$
Y_{r}(y)=\left(\begin{array}{ccc}
1 & a^{T} & b_{r}^{T}  \tag{24}\\
a & A & B_{r} \\
b_{r} & B_{r} & B_{r}
\end{array}\right)
$$

where $A:=\left(y_{i j}\right)_{i, j \in \mathcal{V}}, B_{r}:=\left(y_{\{i, j, r\}}\right)_{i, j \in \mathcal{V}}$ are symmetric $\mathcal{V} \times \mathcal{V}$ matrices, and $a:=\left(y_{i}\right)_{i \in \mathcal{V}}$, $b_{r}:=\left(y_{i r}\right)_{i \in \mathcal{V}}$. As $b_{r}$ coincides with the $r$-th column of $A$ and of $B_{r}$, by applying some column/row manipulation to $Y_{r}(y)$, one deduces that

$$
Y_{r}(y) \succeq 0 \Longleftrightarrow B_{r} \succeq 0 \text { and } \tilde{C}_{r}:=\left(\begin{array}{cc}
1-y_{r} & a^{T}-b_{r}^{T}  \tag{25}\\
a-b_{r} & A-B_{r}
\end{array}\right) \succeq 0
$$

which permits to reduce the size of the matrices involved in program (23). Setting

$$
\begin{aligned}
& \mathrm{TH}(\mathcal{G})=\left\{x \in \mathbb{R}^{\mathcal{P}_{1}(\mathcal{V})} \mid \exists y \in \mathbb{R}^{\mathcal{P}_{2}(\mathcal{V})} \text { s.t. } M_{1}(y) \succeq 0, y_{i j}=0(i j \in \mathcal{E}), x_{I}=y_{I}\left(I \in \mathcal{P}_{1}(\mathcal{V})\right)\right\}, \\
& N_{+}(\mathrm{TH}(\mathcal{G}))=\left\{x \in \mathbb{R}^{\mathcal{V}} \mid \exists y \in \mathbb{R}^{\mathcal{P}_{2}(\mathcal{V})}\right. \text { s.t. } M_{1}(y) \succeq 0, y_{\emptyset}=1, x_{i}=y_{i}(i \in \mathcal{V}), \\
&\left.\left(y_{I \cup\{r\}}\right)_{I \in \mathcal{P}_{1}(\mathcal{V})},\left(y_{I}-y_{I \cup\{r\}}\right)_{I \in \mathcal{P}_{1}(\mathcal{V})} \in \mathrm{TH}(\mathcal{G})\right\}
\end{aligned}
$$

one can verify that

$$
\begin{equation*}
\ell(\mathcal{G}) \leq \max _{x \in N_{+}(\mathrm{TH}(\mathcal{G}))} \sum_{i \in \mathcal{V}} x_{i} \tag{26}
\end{equation*}
$$

To see it, let $y$ be feasible for (23); then $x:=\left(y_{i}\right)_{i \in \mathcal{V}} \in N_{+}(\mathrm{TH}(\mathcal{G}))$. Indeed, the vector $\left(y_{I \cup\{r\}}\right)_{I \in \mathcal{P}_{1}(V)}$ is equal to the first column of the principal submatrix of $Y_{r}(y)$ indexed by $\{r\} \cup\{\{r, i\} \mid i \in \mathcal{V}\}$, and $\left(y_{I}-y_{I \cup\{r\}}\right)_{I \in \mathcal{P}_{1}(V)}$ is the first column of the matrix $\tilde{C}_{r}$ in (25).
3.2. The semidefinite programming bounds $\ell^{(k)}(\mathcal{G})$ for the coding problem. Let $G$ be a group of automorphisms of the graph $\mathcal{G}=(\mathcal{V}, \mathcal{E})$; that is, $G \subseteq \operatorname{Sym}(\mathcal{V})$ and each $\sigma \in G$ preserves edges, i.e., $i j \in \mathcal{E} \Longrightarrow \sigma(i) \sigma(j) \in \mathcal{E}$. Then $G$ acts on the set $\mathcal{P}_{k}(\mathcal{V})$ indexing matrices in the program (22), by letting $\sigma(I)=\{\sigma(i) \mid i \in I\}$ for $\sigma \in G$, $I \in \mathcal{P}_{k}(\mathcal{V})$.

Lemma 7. Let $G$ be a group of automorphisms of $\mathcal{G}$. Then the program (22) is invariant under the action of $G$.

Proof. Set $Y=M_{k}(y)$. The objective function is of the form $\sum_{i \in \mathcal{V}} y_{i}=\sum_{i \in \mathcal{V}} Y_{i, i}=$ $\langle C, Y\rangle$, where $C$ is invariant under action of $G$, since the set $\{(\{i\},\{i\}) \mid i \in \mathcal{V}\}$ is a union of orbits of $\mathcal{P}_{k}(\mathcal{V}) \times \mathcal{P}_{k}(\mathcal{V})$ (in fact, a single orbit if $G$ is vertex-transitive). The constraint $y_{\emptyset}=Y_{\emptyset, \emptyset}=1$ is of the form $\langle A, Y\rangle=1$ where $A$ is invariant, since the set $\{(\emptyset, \emptyset)\}$ is an orbit. The class of edge constraints (19) is invariant under action of $G$ : If $I \cup J$ contains an edge $i j$ and $\sigma \in G$, then $\sigma(I) \cup \sigma(J)$ contains the edge $\sigma(i) \sigma(j)$ and thus the equation: $y_{\sigma(I) \sigma(J)}=Y_{\sigma(I), \sigma(J)}=0$ is again an edge constraint. Similarly, the class of moment constraints (18) is also invariant under action of $G$.

By Corollary 2, the parameter $\ell^{(k)}(\mathcal{G})$ can therefore be formulated as the optimum of a semidefinite program in $N$ variables involving $N \times N$ matrices, where $N$ is the number of orbits of the set $\mathcal{P}_{k}(\mathcal{V}) \times \mathcal{P}_{k}(\mathcal{V})$ under the action of the group $G$. We now apply this technique to the graph $\mathcal{G}=\mathcal{G}(n, d)$ and to the group $G=\operatorname{Aut}(\mathcal{P})$, the group of automorphisms of $\mathcal{P}$ (introduced in (10)). Recall that $\mathcal{G}(n, d)$ has node set $\mathcal{P}$, the collection of subsets of $\{1, \ldots, n\}$, with an edge $(I, J)$ if $|I \Delta J| \in\{1, \ldots, d-1\}$ for $I, J \in \mathcal{P}$. Thus $G$ also acts on the set $\mathcal{P}_{k}(\mathcal{P})=\{\mathcal{A} \subseteq \mathcal{P}| | \mathcal{A} \mid \leq k\}$, indexing the matrix variable in program (22). We show:

THEOREM 8. For any fixed $k$, one can compute (to an arbitrary precision) the parameter $\ell^{(k)}(\mathcal{G}(n, d))$ from (22) in time polynomial in $n$. The same holds for the parameter $\ell_{+}^{(k)}(\mathcal{G})$ obtained by adding the constraints (21) to (22).
Proof. Let $k$ be fixed and let $N_{k}$ denote the number of orbits of the set $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ under the action of the group $G$. As mentioned above, the parameter $\ell^{(k)}(\mathcal{G}(n, d))$ can be expressed via a semidefinite program of the form (8), involving $N_{k} \times N_{k}$ matrices and $N_{k}$ variables. Hence, to show Theorem 8, it suffices to verify that $N_{k}$ is bounded by a polynomial in $n$ and that the new program equivalent to (22) can be constructed in time polynomial in $n$.

To begin with, it is useful to have a way to identify the orbits of the set $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$.
Consider $(\mathcal{A}, \mathcal{B}) \in \mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ with $r:=|\mathcal{A}|$ and $s:=|\mathcal{B}|$. If $r=s=0$ then $\mathcal{A}=\mathcal{B}=\emptyset$, the empty subset of $\mathcal{P}$, and the orbit of $(\emptyset, \emptyset)$ just consists of the pair $(\emptyset, \emptyset)$. We can now assume that $r+s \geq 1$. Let $\overrightarrow{\mathcal{A}}=\left(A_{1}, \ldots, A_{r}\right)$ be an ordering of the elements
of $\mathcal{A}$; similarly, $\overrightarrow{\mathcal{B}}=\left(B_{1}, \ldots, B_{s}\right)$ is an ordering of the elements of $\mathcal{B}$. Then one can define the $(r+s) \times n$ incidence tableau of $(\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}})$, whose rows are the incidence vectors $\chi^{A_{1}}, \ldots, \chi^{A_{r}}, \chi^{B_{1}}, \ldots, \chi^{B_{s}}$ (in that order) of the sets $A_{1}, \ldots, A_{r}, B_{1}, \ldots, B_{s}$. Define the function $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}:\{0,1\}^{r} \times\{0,1\}^{s} \longrightarrow \mathbb{Z}_{+}$where, for $(u, v) \in\{0,1\}^{r} \times\{0,1\}^{s}, \varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}(u, v)$ is the multiplicity of $(u, v)$ as a column of the incidence tableau of $(\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}})$. Thus $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}$ belongs to the set $\Phi_{r, s}$ consisting of the functions $\phi:\{0,1\}^{r} \times\{0,1\}^{s} \longrightarrow\{0,1, \ldots, n\}$ satisfying: $\sum_{u \in\{0,1\}^{r}, v \in\{0,1\}^{s}} \phi(u, v)=n$ and, for all $i \neq j \in\{1, \ldots, r\}$ (resp., $i \neq j \in\{1, \ldots, s\}$ ), there exists $(u, v) \in\{0,1\}^{r} \times\{0,1\}^{s}$ for which $\phi(u, v) \geq 1$ and $u_{i} \neq u_{j}\left(\right.$ resp., $\left.v_{i} \neq v_{j}\right)$.

Let $\overrightarrow{\mathcal{A}^{\prime}}$ (resp., $\overrightarrow{\mathcal{B}^{\prime}}$ ) be another ordered sequence of $r$ (resp., of $s$ ) distinct elements of $\mathcal{P}$ and let $\phi=\phi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}, \phi^{\prime}=\varphi_{\overrightarrow{\mathcal{A}^{\prime}}, \overrightarrow{\mathcal{B}^{\prime}}}$. Then, $\overrightarrow{\mathcal{\mathcal { A }}^{\prime}}=\left(\sigma\left(A_{1}\right), \ldots, \sigma\left(A_{r}\right)\right)$ and $\overrightarrow{\mathcal{B}^{\prime}}=\left(\sigma\left(B_{1}\right), \ldots, \sigma\left(B_{s}\right)\right)$ for some $\sigma \in G$ if and only if $\phi(u, v)+\phi(\mathbf{1}-u, \mathbf{1}-v)=\phi^{\prime}(u, v)+\phi^{\prime}(\mathbf{1}-u, \mathbf{1}-v)$ for all $(u, v) \in\{0,1\}^{r} \times\{0,1\}^{s}$. (Here, $\mathbf{1}:=(1, \ldots, 1)$ denotes the all-ones vector of the suitable size.) Moreover, $\overrightarrow{\mathcal{A}^{\prime}}=\left(A_{\alpha(1)}, \ldots, A_{\alpha(r)}\right)$ and $\overrightarrow{\mathcal{B}^{\prime}}=\left(B_{\beta(1)}, \ldots, B_{\beta(s)}\right)$ for some permutations $\alpha \in \operatorname{Sym}(r), \beta \in \operatorname{Sym}(s)$ if and only if $\phi^{\prime}(u, v)=\phi(\alpha(u), \beta(v))$ for all $(u, v) \in\{0,1\}^{r} \times\{0,1\}^{s}$, setting $\alpha(u):=\left(u_{\alpha(1)}, \ldots, u_{\alpha(r)}\right), \beta(v):=\left(v_{\beta(1)}, \ldots, v_{\beta(s)}\right)$. For two elements $\phi, \phi^{\prime} \in \Phi_{r, s}$, write $\phi \sim \phi^{\prime}$ if
$\left.\phi^{\prime}(u, v)+\phi^{\prime}(\mathbf{1}-u, \mathbf{1}-v)=\phi(\alpha(u), \beta(v))+\phi(\mathbf{1}-\alpha(u), \mathbf{1}-\beta(v))\right) \forall(u, v) \in\{0,1\}^{r} \times\{0,1\}^{s}$ for some $\alpha \in \operatorname{Sym}(r), \beta \in \operatorname{Sym}(s)$. This defines an equivalence relation on $\Phi_{r, s}$.

We can now characterize orbits in the following way: Two pairs $(\mathcal{A}, \mathcal{B}),\left(\mathcal{A}^{\prime}, \mathcal{B}^{\prime}\right)$ belong to the same orbit of $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ under action of $G$ if and only if $|\mathcal{A}|=\left|\mathcal{A}^{\prime}\right|=: r$, $|\mathcal{B}|=\left|\mathcal{B}^{\prime}\right|=$ : s and $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}} \sim \varphi_{\overrightarrow{\mathcal{A}^{\prime}}, \overrightarrow{\mathcal{B}^{\prime}}}$ for some respective orderings $\overrightarrow{\mathcal{A}} \overrightarrow{\mathcal{B}}, \overrightarrow{\mathcal{A}^{\prime}}, \overrightarrow{\mathcal{B}^{\prime}}$ of $\mathcal{A}, \mathcal{B}, \mathcal{A}^{\prime}$, $\mathcal{B}^{\prime}$. Thus each orbit of $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ corresponds to an equivalence class of $\cup_{0 \leq r, s \leq k} \Phi_{r, s}$. Hence the number $N_{k}$ of orbits of $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ is at most $1+\sum_{\substack{0 \leq r, s \leq k \\ r+s \geq 1}}(n+1)^{2^{r \mp s-1}-1}$, giving:

$$
\begin{equation*}
N_{k} \leq O\left(n^{2^{2 k-1}-1}\right) \tag{27}
\end{equation*}
$$

We now verify that the matrices $L_{i}\left(i=1, \ldots, N_{k}\right)$ (as defined in (5)) can be constructed in time polynomial in $n$.

For this one first needs to be able to compute in time polynomial in $n$ the cardinality of the orbits of $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$. Given $\phi_{0} \in \Phi_{r, s}(0 \leq r, s \leq k, r+s \geq 1)$, one has to count the number $L_{\phi_{0}}$ of pairs $(\mathcal{A}, \mathcal{B}) \in \mathcal{P}_{=r}(\mathcal{P}) \times \mathcal{P}_{=s}(\mathcal{P})$ for which $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}} \sim \phi_{0}$ for some orderings $\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}$ of $\mathcal{A}, \mathcal{B}$. Given $\phi \sim \phi_{0}$, there are $\ell_{\phi}:=n!/ \prod_{\substack{u \in\{0,1\}^{r} \\ v \in\{0,1\}^{s}}} \phi(u, v)$ ! pairs $(\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}})$ for which $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}=\phi_{0}$. Therefore, $L_{\phi_{0}}=\frac{1}{r!s!} \sum_{\phi \sim \phi_{0}} \ell_{\phi}$, which can be computed in time polynomial in $n$ since one can enumerate the equivalence class of $\phi_{0}$ in time polynomial in $n$.

Next we verify that one can compute in time polynomial in $n$ the multiplication parameters $\gamma_{i, j}^{k}$ from (4), used for defining the matrices $L_{i}$ in (5). For this, given $(\mathcal{A}, \mathcal{B}) \in$ $\mathcal{P}_{=r}(\mathcal{P}) \times \mathcal{P}_{=s}(\mathcal{P})$ with respective orderings $\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}$, given an integer $0 \leq t \leq k$, and given $\phi_{0} \in \Phi_{r, t}, \psi_{0} \in \Phi_{s, t}$, one has to count the number $L_{\phi_{0}, \psi_{0}}$ of elements $\mathcal{C} \in \mathcal{P}_{=t}(\mathcal{P})$ for which $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{C}}} \sim \phi_{0}$ and $\varphi_{\overrightarrow{\mathcal{B}}, \overrightarrow{\mathcal{C}}} \sim \psi_{0}$ for some ordering $\overrightarrow{\mathcal{C}}$ of $\mathcal{C}$. Set $\xi:=\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}}$. Given $\phi \sim \phi_{0}$ and $\psi \sim \psi_{0}$, we first count the number $\ell_{\phi, \psi}$ of ordered sequences $\overrightarrow{\mathcal{C}}$ of $t$ elements of
$\mathcal{P}$ for which $\varphi_{\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{C}}}=\phi$ and $\varphi_{\overrightarrow{\mathcal{B}}, \overrightarrow{\mathcal{C}}}=\psi$. For this let $x(u, v, w)$ denote the multiplicity of $(u, v, w) \in\{0,1\}^{r} \times\{0,1\}^{s} \times 2^{t}$ as column of the incidence tableau of $(\overrightarrow{\mathcal{A}}, \overrightarrow{\mathcal{B}}, \overrightarrow{\mathcal{C}})$. The first $r+s$ rows of the tableau are given and one needs to determine its last $t$ rows. Then, $x(u, v, w) \in\{0,1, \ldots, n\}$ satisfy the system

$$
\begin{array}{ll}
\sum_{v \in\{0,1\}^{s}} x(u, v, w)=\phi(u, w) & \forall u \in\{0,1\}^{r}, w \in\{0,1\}^{t} \\
\sum_{u \in\{0,1\}^{r}} x(u, v, w)=\psi(v, w) & \forall v \in\{0,1\}^{s}, w \in\{0,1\}^{t}  \tag{28}\\
\sum_{w \in\{0,1\}^{t}} x(u, v, w)=\xi(u, v) & \forall u \in\{0,1\}^{r}, v \in\{0,1\}^{s} .
\end{array}
$$

As the system (28) has polynomially many variables and equations, its set $S$ of solutions can be found by complete enumeration and $|S| \leq(n+1)^{2^{r+s+t}}$. Therefore, $\ell_{\phi, \psi}=$ $\sum_{x \in S} \sum_{u \in\{0,1\}^{r}, v \in\{0,1\}^{s}} \frac{\xi(u, v)!}{\prod_{w \in 2^{t} x(u, v, w)!}}$, the number of possible ways to assign the vectors $w \in 2^{t}$ as columns of the lower $t \times n$ part of the tableau. Now, $L_{\phi_{0}, \psi_{0}}=\frac{1}{t!} \sum_{\substack{\phi \sim 0_{0} \\ \psi \sim \psi_{0}}} \ell_{\phi, \psi}$ can be computed in time polynomial in $n$ since one can enumerate the equivalence classes of $\phi_{0}$ and $\psi_{0}$.

Remains only to construct the linear constraints corresponding to the moment constraints (18) and the edge constraints (19). Label the orbits of $\mathcal{P}_{k}(\mathcal{P}) \times \mathcal{P}_{k}(\mathcal{P})$ as $\mathcal{O}_{1}, \ldots, \mathcal{O}_{N_{k}}$ and determine a pair $\left(\mathcal{A}_{i}, \mathcal{B}_{i}\right)$ belonging to each orbit $\mathcal{O}_{i}$. Then the moment constraints read: $x_{i}=x_{j}$ if $\mathcal{A}_{i} \cup \mathcal{B}_{i}=\sigma\left(\mathcal{A}_{j} \cup \mathcal{B}_{j}\right)$ for some $\sigma \in G$ (which can be tested in time polynomial in $n$ ), and the edge constraints read: $x_{i}=0$ if $\mathcal{A}_{i} \cup \mathcal{B}_{i}$ contains a pair ( $I, J$ ) with $|I \Delta J| \in\{1, \ldots, d-1\}$.

The bounds (21) become: $x_{i} \geq 0\left(i=1, \ldots, N_{k}\right)$ and $x_{i} \leq x_{j}$ if $\mathcal{A}_{i} \cup \mathcal{B}_{i} \supseteq \sigma\left(\mathcal{A}_{j} \cup \mathcal{B}_{j}\right)$ for some $\sigma \in G$ (which can be tested in time polynomial in $n$ ).

Therefore, the parameter $\ell^{(k)}(\mathcal{G}(n, d))$ (or $\left.\ell_{+}^{(k)}(\mathcal{G}(n, d))\right)$ can be computed as the optimum value of a semidefinite program of the form (8) involving $N_{k} \times N_{k}$ matrices, with $N_{k}$ variables and $O\left(N_{k}^{2}\right)$ linear constraints. As $N_{k}=O\left(n^{2^{2 k-1}-1}\right)$, it can be computed in time polynomial in $n$ (to any precision), which concludes the proof of Theorem 8.

The result from Theorem 8 is mainly of theoretical value for $k \geq 2$. Indeed, for $k=2$, $N_{k}=O\left(n^{7}\right)$ and thus the semidefinite program defining $\ell^{(2)}(\mathcal{G}(n, d))$ is already too large to be solved in practice for interesting values of $n$ by the currently available software for semidefinite programming.
3.3. Refining Schrijver's bound. We begin with observing that, when a graph $\mathcal{G}$ has a vertex-transitive group $G$ of automorphisms then, in the program (23), it suffices to require the condition $Y_{r}(y) \succeq 0$ for one choice of $r \in \mathcal{V}$.

Lemma 9. Let $G$ be a group of automorphisms of the graph $\mathcal{G}=(\mathcal{V}, \mathcal{E})$. The program (23) is invariant under action of $G$. If $G$ is vertex-transitive then, in (23), it suffices to require the constraint $Y_{r}(y) \succeq 0$ for one choice of $r \in \mathcal{V}$ (instead of for all $r \in \mathcal{V}$ ).

Proof. The first part of the proof is analogous to the proof of Lemma 7. Here, we use the fact that, for $r \in \mathcal{V}, \sigma \in G, Y_{r}(\sigma(y))=\sigma\left(Y_{\sigma(r)}(y)\right)$. Hence, if $y$ is invariant under action
of $G$, then $Y_{r}(y) \succeq 0$ for some $r \in \mathcal{V}$ implies that $Y_{r}(y) \succeq 0$ for all $r \in \mathcal{V}$.
3.3.1. A compact semidefinite formulation for the bound $\ell(\mathcal{G}(n, d))$. In this section we consider the graph $\mathcal{G}=\mathcal{G}(n, d)$ and the group $G=\operatorname{Aut}(\mathcal{P})$, whose action on the graph $\mathcal{G}(n, d)$ is indeed vertex-transitive. We set:

$$
\begin{equation*}
\mathcal{X}:=\mathcal{P}_{2}(\mathcal{P} ; \emptyset)=\{\emptyset\} \cup\{\{I\} \mid I \in \mathcal{P}\} \cup\{\{\emptyset, I\} \mid I \in \mathcal{P}\} \tag{29}
\end{equation*}
$$

Applying Lemma 9, one can reformulate the parameter $\ell(\mathcal{G}(n, d))$ as

$$
\begin{array}{cl}
\ell(\mathcal{G}(n, d))=\max & \sum_{I \in \mathcal{P}} y_{\{I\}} \\
\text { s.t. } & Y(y) \succeq 0, y_{\emptyset}=1,  \tag{30}\\
& y_{\{I, J\}}=0 \text { if }|I \Delta J| \in\{1, \ldots, d-1\} \\
& y_{\mathcal{A}}=y_{\sigma(\mathcal{A})} \text { for } \sigma \in G, \mathcal{A} \in \mathcal{X}
\end{array}
$$

where the matrix variable $Y(y)$ is indexed by the set $\mathcal{X}$ and satisfies: $Y(y)_{\mathcal{A}, \mathcal{B}}=y_{\mathcal{A} \cup \mathcal{B}}$ for $\mathcal{A}, \mathcal{B} \in \mathcal{X}$. By $(24), Y(y)$ has the form

$$
Y(y)=\left(\begin{array}{ccc}
1 & a^{T} & b^{T}  \tag{31}\\
a & A & B \\
b & B & B
\end{array}\right)
$$

with $A=\left(y_{\{I, J\}}\right)_{I, J \in \mathcal{P}}, B=\left(y_{\{\emptyset, I, J\}}\right)_{I, J \in \mathcal{P}}, a=\left(y_{\{I\}}\right)_{I \in \mathcal{P}}$, and $b=\left(y_{\{\emptyset, I\}}\right)_{I \in \mathcal{P}}$. As $y$ is invariant under action of $G$, it follows that $A_{I, J}=A_{I^{\prime}, J^{\prime}}$ if $I^{\prime}=\sigma(I), J^{\prime}=\sigma(J)$ for some $\sigma \in G$, i.e., if $|I \Delta J|=\left|I^{\prime} \Delta J^{\prime}\right|$. That is, the matrix $A$ belongs to the Bose-Mesner algebra $\mathcal{B}_{n}$; say,

$$
\begin{equation*}
A=\sum_{k=0}^{n} x_{k} M_{k} \text { for some real scalars } x_{0}, \ldots, x_{n} \tag{32}
\end{equation*}
$$

where the matrices $M_{k}$ are as in (11). Moreover, $B_{I, J}=B_{I^{\prime}, J^{\prime}}$ if $I^{\prime}=\sigma(I), J^{\prime}=\sigma(J)$, $\emptyset=\sigma(\emptyset)$ for some $\sigma \in G$, i.e., if $\left|I^{\prime}\right|=|I|,\left|J^{\prime}\right|=|J|$ and $|I \cap J|=\left|I^{\prime} \cap J^{\prime}\right|$. That is, the matrix $B$ belongs to the Terwilliger algebra $\mathcal{A}_{n}$; say,

$$
\begin{equation*}
B=\sum_{i, j, t \geq 0} x_{i, j}^{t} M_{i, j}^{t} \text { for some real scalars } x_{i, j}^{t} \tag{33}
\end{equation*}
$$

where the matrices $M_{i, j}^{t}$ are as in (9) and $x_{i, j}^{t}=x_{j, i}^{t}$ for all $i, j, t$. The variables $x_{k}$ and $x_{i, j}^{t}$ are related by

$$
\begin{equation*}
x_{k}=x_{0, k}^{0} \text { for } k=0,1, \ldots, n \tag{34}
\end{equation*}
$$

(since $x_{k}=A_{\emptyset, I}=B_{\emptyset, I}=x_{0, k}^{k}$ for $|I|=k$ ). Moreover,

$$
\begin{equation*}
x_{i, j}^{t}=x_{i^{\prime}, j^{\prime}}^{t^{\prime}} \text { if }\left(i^{\prime}, j^{\prime}, i^{\prime}+j^{\prime}-2 t^{\prime}\right) \text { is a permutation of }(i, j, i+j-2 t) . \tag{35}
\end{equation*}
$$

Equivalently, $x_{i, j}^{t}=x_{i+j-2 t, i}^{i-t}=x_{i+j-2 t, j}^{j-t}$. (Indeed, let $I, J \in \mathcal{P}$ with $i=|I|, j=|J|$, $t=|I \cap J| . \quad$ As $\sigma:=s_{J} \operatorname{maps} \mathcal{A}:=\{\emptyset, I, J\}$ to $\{\emptyset, J, I \Delta J\}$ and $y_{\sigma(\mathcal{A})}=y_{\mathcal{A}}$, then $\left.x_{i, j}^{t}=y_{\{\emptyset, I, J\}}=y_{\{\emptyset, J, I \Delta J\}}=x_{j, i+j-2 t}^{j-t}.\right)$ The edge inequalities become:

$$
\begin{equation*}
x_{i, j}^{t}=0 \text { if }\{i, j, i+j-2 t\} \cap\{1, \ldots, d-1\} \neq \emptyset \tag{36}
\end{equation*}
$$

and the bounds (21) read:

$$
\begin{equation*}
0 \leq x_{i, j}^{t} \leq x_{i, 0}^{0} \text { for } i, j, t=0, \ldots, n \tag{37}
\end{equation*}
$$

From (25), we know that $Y(y) \succeq 0$ if and only if

$$
B=\sum_{i, j, t=0}^{n} x_{i, j}^{t} M_{i, j}^{t} \succeq 0 \text { and } \tilde{C}:=\left(\begin{array}{cc}
1-x_{0,0}^{0} & c^{T} \\
c & C
\end{array}\right) \succeq 0
$$

where

$$
C:=A-B=\sum_{i, j, t=0}^{n}\left(x_{0, i+j-2 t}^{0}-x_{i, j}^{t}\right) M_{i, j}^{t} \text { and } c:=a-b=\sum_{i=0}^{n}\left(x_{0,0}^{0}-x_{0, i}^{0}\right) \chi^{\mathcal{P}=i(V)} .
$$

(Recall $\mathcal{P}_{=i}(V)=\{I \subseteq V| | I \mid=i\}$.) Thus $\tilde{C}$ is of the form (16). For $k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$, define the matrices:

$$
\begin{equation*}
A_{k}(x):=\left(\sum_{t}\binom{n-2 k}{i-k}^{-\frac{1}{2}}\binom{n-2 k}{j-k}^{-\frac{1}{2}} \beta_{i, j, k}^{t} x_{0, i+j-2 t}^{0}\right)_{i, j=k}^{n-k} \tag{38}
\end{equation*}
$$

and $B_{k}(x)$ as in (13), where $\beta_{i, j, k}^{t}$ are as in (14). It follows from Lemma 6 that the positive semidefiniteness of $Y(y)$ is equivalent to
(i) $\quad B_{k}(x) \succeq 0$ for $k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$
(ii) $\quad A_{k}(x)-B_{k}(x) \succeq 0$ for $k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$

$$
\text { (iii) } \quad\left(\begin{array}{cc}
1-x_{0,0}^{0} & \tilde{c}^{T}  \tag{39}\\
\tilde{c} & A_{0}(x)-B_{0}(x)
\end{array}\right) \succeq 0, \quad \text { setting } \tilde{c}:=\left(\binom{n}{i}^{\frac{1}{2}}\left(x_{0,0}^{0}-x_{0, i}^{0}\right)\right)_{i=0}^{n} .
$$

(Of course, (39)(iii) implies (ii) for $k=0$.) Summarizing, we have shown:

$$
\ell(\mathcal{G}(n, d))=\max 2^{n} x_{0,0}^{0} \quad \text { s.t. } \quad x_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy }
$$

$$
\begin{equation*}
(35),(36),(39)(i)-(i i i) \tag{40}
\end{equation*}
$$

Similarly,

$$
\begin{align*}
\ell_{+}(\mathcal{G}(n, d))=\max 2^{n} x_{0,0}^{0} \text { s.t. } \quad & x_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy }  \tag{41}\\
& (35),(36),(37),(39)(i)-(i i i) .
\end{align*}
$$

Hence both parameters can be computed via a semidefinite program of size $O\left(n^{3}\right)$.
3.3.2. Comparison with Schrijver's bound. Schrijver [13] introduced the following upper bound for the stability number $A(n, d)$ of the graph $\mathcal{G}(n, d)$ :

$$
\begin{align*}
\ell_{s c h}(\mathcal{G}(n, d)):=\max & \sum_{i=0}^{n}\binom{n}{i} x_{0, i}^{0}  \tag{42}\\
\text { s.t. } \quad & x_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy }(35),(36),(37), \\
& (39)(i)-(i i) \text { and } x_{0,0}^{0}=1
\end{align*}
$$

As noted in [13], Schrijver's bound is at least as good as the Delsarte bound, which coincides with $\vartheta^{\prime}(\mathcal{G}(n, d))=\ell_{+}^{(1)}(\mathcal{G}(n, d))$. We now show:
Lemma 10. The bound $\ell_{+}(\mathcal{G}(n, d))$ is at least as good as $S$ chrijver's bound $\ell_{\text {sch }}(\mathcal{G}(n, d))$ from (42); that is, $\ell_{+}(\mathcal{G}(n, d)) \leq \ell_{s c h}(\mathcal{G}(n, d))$.

Proof. Let $\left(x_{i, j}^{t}\right)_{i, j, t=0}^{n}$ be feasible for the program (41). Define $y_{i, j}^{t}:=x_{i, j}^{t} / x_{0,0}^{0}$ for all $i, j, t=0, \ldots, n$. Then the variables $y_{i, j}^{t}$ satisfy (35), (36), (37), (39) (i)-(ii), and $y_{0,0}^{0}=1$. Remains to verify that $2^{n} x_{0,0}^{0} \leq \sum_{i=0}^{n}\binom{n}{i} y_{0, i}^{0}$, i.e., $2^{n}\left(x_{0,0}^{0}\right)^{2} \leq \sum_{i=0}^{n}\binom{n}{i} x_{0, i}^{0}$. For this, recall that the conditions (39) (i)-(iii) are equivalent to the positive semidefiniteness of the matrix in (31). In particular, they imply

$$
\left(\begin{array}{cc}
1 & a^{T} \\
a & A
\end{array}\right) \succeq 0, \quad \text { i.e., } A-a a^{T} \succeq 0
$$

where $A$ is as in (32), $a^{T}=\left(x_{0,0}^{0}, \ldots, x_{0,0}^{0}\right), x_{k}=x_{0, k}^{0}$ for $k=0, \ldots, n$. Thus, $a a^{T}=$ $\left(x_{0,0}^{0}\right)^{2} J$, where $J$ is the all-ones matrix. As $A-\left(x_{0,0}^{0}\right)^{2} J \succeq 0$, we deduce that $\langle J, A\rangle \geq$ $\left(x_{0,0}^{0}\right)^{2}\langle J, J\rangle=\left(x_{0,0}^{0} 2^{n}\right)^{2}$. But $\langle J, A\rangle=\sum_{k=0}^{n} x_{k}\left\langle J, M_{k}\right\rangle=\sum_{k=0}^{n} x_{k} 2^{n}\binom{n}{k}$, which gives $\sum_{k=0}^{n} x_{0, k}^{0}\binom{n}{k} \geq 2^{n}\left(x_{0,0}^{0}\right)^{2}$.
3.3.3. Refining the bound $\ell_{+}(\mathcal{G}(n, d))$. It is possible to define a new bound $\ell_{++}(\mathcal{G}(n, d))$, at least as good as the bound $\ell_{+}(\mathcal{G}(n, d))$, whose computation still involves a semidefinite program of size $O\left(n^{3}\right)$. Namely, let us now consider as matrix variable the principal submatrix $Y(y)$ of $M_{2}(y)$ indexed by the set

$$
\begin{equation*}
\mathcal{X}_{+}:=\{\emptyset\} \cup\{\{I\} \mid I \in \mathcal{P}\} \cup\{\{\emptyset, I\} \mid I \in \mathcal{P}\} \cup\{\{I, V\} \mid I \in \mathcal{P}\} \tag{43}
\end{equation*}
$$

Then, $Y(y)$ has the block structure:

$$
Y(y)=\left(\begin{array}{cccc}
1 & a^{T} & b^{T} & c^{T}  \tag{44}\\
a & A & B & C \\
b & B & B & D \\
c & C & D & C
\end{array}\right)
$$

where $A=\left(y_{\{I, J\}}\right)_{I, J \in \mathcal{P}}, B=\left(y_{\{\emptyset, I, J\}}\right)_{I, J \in \mathcal{P}}, C=\left(y_{\{I, J, V\}}\right)_{I, J \in \mathcal{P}}, D=\left(y_{\{\emptyset, I, J, V\}}\right)_{I, J \in \mathcal{P}}$, $a=\left(y_{\{I\}}\right)_{I \in \mathcal{P}}, b=\left(y_{\{\emptyset, I\}}\right)_{I \in \mathcal{P}}$, and $c=\left(y_{\{I, V\}}\right)_{I \in \mathcal{P}}$. The matrices $A, B$ are given by (32), (33). The matrix $C$ is a permutation of $B$; namely,

$$
C=\sum_{i, j, t=0}^{n} x_{n-i, n-j}^{n+t-i-j} M_{i, j}^{t}
$$

The matrix $D$ too belongs to the Terwilliger algebra:

$$
D=\sum_{i, j, t=0}^{n} z_{i, j}^{t} M_{i, j}^{t} \text { for some real scalars } z_{i, j}^{t}
$$

satisfying $z_{i, j}^{t}=z_{j, i}^{t}$; indeed, $D_{I, J}=D_{I^{\prime}, J^{\prime}}$ if there exists $\sigma \in G$ such that $\sigma(\emptyset)=\emptyset$, $\sigma(I)=I^{\prime}, \sigma(J)=J^{\prime}$ (then $\sigma(V)=V$ ), i.e., if $|I|=\left|I^{\prime}\right|,|J|=\left|J^{\prime}\right|,|I \cap J|=\left|I^{\prime} \cap J^{\prime}\right|$. We have the following relations for the variables $x_{i, j}^{t}, z_{i, j}^{t}$ :

$$
\begin{equation*}
z_{i, j}^{t}=z_{n-i, n-j}^{n+t-i-j} \text { for all } i, j, t=0, \ldots, n \tag{45}
\end{equation*}
$$

since $D_{I, J}=y_{\{\emptyset, V, I, J\}}=y_{\{\emptyset, V, V \Delta I, V \Delta J\}}=D_{V \Delta I, V \Delta J}$, and

$$
\begin{equation*}
z_{i, i}^{i}=z_{0, i}^{0}=z_{n, i}^{i}=x_{i, n}^{i} \quad \text { for } i=0, \ldots, n \tag{46}
\end{equation*}
$$

since $y_{\{\emptyset, V, I\}}=D_{I, I}=D_{\emptyset, I}=D_{V, I}=B_{V, I}$. The edge condition for the $z$-variables reads:

$$
\begin{equation*}
z_{i, j}^{t}=0 \text { if }\{i, j, n-i, n-j, i+j-2 t\} \cap\{1, \ldots, d-1\} \neq 0 \text { for } i, j, t=0, \ldots, n \tag{47}
\end{equation*}
$$

The bounds (21) imply:

$$
\begin{equation*}
0 \leq z_{i, j}^{t} \leq x_{i, j}^{t}, \quad z_{i, j}^{t} \leq z_{i, i}^{i} \text { for } i, j, t=0, \ldots, n \tag{48}
\end{equation*}
$$

As each non-border block of the matrix $Y(y)$ in (44) belongs to the Terwilliger algebra, one can block-diagonalize $Y(y)$. Indeed, each non-border block in the matrix

$$
\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & U^{T} & 0 & 0 \\
0 & 0 & U^{T} & 0 \\
0 & 0 & 0 & U^{T}
\end{array}\right) Y(y)\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & U & 0 & 0 \\
0 & 0 & U & 0 \\
0 & 0 & 0 & U
\end{array}\right)=\left(\begin{array}{cccc}
1 & a^{T} U & b^{T} U & c^{T} U \\
U a & U^{T} A U & U^{T} B U & U^{T} C U \\
U b & U^{T} B U & U^{T} B U & U^{T} D U \\
U c & U^{T} C U & U^{T} D U & U^{T} C U
\end{array}\right)
$$

is block-diagonal with respect to the same partition, with $\left\lfloor\frac{n}{2}\right\rfloor+1$ distinct blocks labeled by $k=0,1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor$. It follows from Lemma 6 that $a^{T} U=\left(\tilde{a}^{T}, 0, \ldots, 0\right), b^{T} U=\left(\tilde{b}^{T}, 0, \ldots, 0\right)$, $c^{T} U=\left(\tilde{c}^{T}, 0, \ldots, 0\right)$, where $\tilde{a}=x_{0,0}^{0} \sum_{i=0}^{n}\binom{n}{i}^{\frac{1}{2}} \chi^{\mathcal{P}=i(V)}, \tilde{b}=\sum_{i=0}^{n} x_{0, i}^{0}\binom{n}{i}^{\frac{1}{2}} \chi^{\mathcal{P}=i(V)}$ and $\tilde{c}=\sum_{i=0}^{n} x_{0, n-i}^{0}\binom{n}{i}^{\frac{1}{2}} \chi^{\mathcal{P}_{=i}(V)}$ are indexed by the positions corresponding to the 0 -th block. Therefore, $Y(y) \succeq 0$ if and only if

$$
\left(\begin{array}{cccc}
1 & \tilde{a}^{T} & \tilde{b}^{T} & \tilde{c}^{T}  \tag{49}\\
\tilde{a} & A_{0} & B_{0} & C_{0} \\
\tilde{b} & B_{0} & B_{0} & D_{0} \\
\tilde{c} & C_{0} & D_{0} & C_{0}
\end{array}\right) \succeq 0, \quad\left(\begin{array}{lll}
A_{k} & B_{k} & C_{k} \\
B_{k} & B_{k} & D_{k} \\
C_{k} & D_{k} & C_{k}
\end{array}\right) \succeq 0 \text { for } k=1, \ldots,\left\lfloor\frac{n}{2}\right\rfloor
$$

where $A_{k}=A_{k}(x)$ is as in (38), $B_{k}=B_{k}(x)$ is as in (13) and

$$
\begin{gathered}
C_{k}=\left(\sum_{t}\binom{n-2 k}{i-k}^{-\frac{1}{2}}\binom{n-2 k}{j-k}^{-\frac{1}{2}} \beta_{i, j, k}^{t} x_{n-i, n-j}^{n+t-i-j}\right)_{i, j=k}^{n-k} \\
D_{k}=\left(\sum_{t}\binom{n-2 k}{i-k}^{-\frac{1}{2}}\binom{n-2 k}{j-k}^{-\frac{1}{2}} \beta_{i, j, k}^{t} z_{i, j}^{t}\right)_{i, j=k}^{n-k}
\end{gathered}
$$

One can now define the bound

$$
\begin{equation*}
\ell_{++}(\mathcal{G}(n, d)):=\max 2^{n} x_{0,0}^{0} \quad \text { s.t. } \quad x_{i, j}^{t}, \quad z_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy } \tag{50}
\end{equation*}
$$

$$
(35),(36),(37),(45),(46),(47),(48),(49)
$$

Obviously,

$$
A(n, d) \leq \ell_{++}(\mathcal{G}(n, d)) \leq \ell_{+}(\mathcal{G}(n, d)) \leq \ell_{s c h}(\mathcal{G}(n, d))
$$

and the bound $\ell_{++}(\mathcal{G}(n, d))$ is again expressed via a semidefinite program of size $O\left(n^{3}\right)$.
Summarizing, the parameters $\ell_{s c h}, \ell_{+}, \ell_{++}$can all be seen as variations of the Lasserre bound $\ell^{(2)}$. Namely, instead of considering the full matrix variable $M_{2}(y)$ indexed by the set $\mathcal{P}_{2}(\mathcal{P})$, one considers a principal submatrix of $M_{2}(y)$ indexed by a subset of $\mathcal{P}_{2}(\mathcal{P})$; namely, by the set $\mathcal{X} \backslash\{\emptyset\}$ for $\ell_{s c h}$, by the set $\mathcal{X}$ for $\ell_{+}$, and by the set $\mathcal{X}_{+}=\mathcal{X} \cup\{\{I, V\} \mid$ $I \in \mathcal{P}\}$ for $\ell_{++}$. (Recall the set $\mathcal{X}$ in (29).)
3.3.4. Reducing the number of variables. The following observation from [13] can be used for reducing the number of variables in the programs $(40),(41),(42),(50)$, and for further refining the corresponding bounds. A well known fact in coding theory is that, if $d$ is odd then $A(n, d)=A(n+1, d+1)$, and if $d$ is even then $A(n, d)$ is attained by a code with all code words having an even Hamming weight. Therefore, it suffices to compute $A(n, d)$ for $d$ even. Moreover, for $d$ even, $A(n, d)=\alpha\left(\mathcal{G}_{e v}(n, d)\right)$, the stability number of the graph $\mathcal{G}_{e v}(n, d)$, defined as the subgraph of $\mathcal{G}(n, d)$ induced by the set

$$
\mathcal{P}_{e v}:=\{I \subseteq V| | I \mid \text { is even }\}
$$

Therefore, for $d$ even, one may add the constraints:

$$
\begin{equation*}
y_{\mathcal{A}}=0 \text { if } \mathcal{A} \nsubseteq \mathcal{P}_{e v} \tag{51}
\end{equation*}
$$

for any $\mathcal{A} \in \mathcal{P}_{2 k}(\mathcal{P})$ to the program (22) defining $\ell^{(k)}(\mathcal{G}(n, d))$, or for any $\mathcal{A} \in \mathcal{P}_{3}(\mathcal{P})$ to the program (23) defining $\ell(\mathcal{G}(n, d))$. Equivalently, one may add the constraints:

$$
\begin{equation*}
x_{i, j}^{t}=0 \text { if one of } i \text { or } j \text { is odd, } \tag{52}
\end{equation*}
$$

to the programs $(40),(41),(42),(50)$, as well as as the constraints:

$$
\begin{equation*}
z_{i, j}^{t}=0 \text { if one of } i, j, \text { or } n \text { is odd } \tag{53}
\end{equation*}
$$

to (50), and the new programs still define upper bounds for $A(n, d)$. Namely, define:

$$
\begin{array}{ll}
\ell^{0}(\mathcal{G}(n, d)):=\max 2^{n} x_{0,0}^{0} \quad \text { s.t. } \quad & x_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy }  \tag{54}\\
& (35),(36),(39)(i)-(i i i),(52)
\end{array}
$$

and let $\ell_{+}^{0}$, (resp., $\ell_{s c h}^{0}, \ell_{++}^{0}$ ) be defined analogously by adding (52) (resp., (52), (52)-(53)) to (41) (resp., (42), (50)).

As $A(n, d)=\alpha\left(\mathcal{G}_{e v}(n, d)\right)$, one may also bound $A(n, d)$ by the parameter $\ell\left(\mathcal{G}_{e v}(n, d)\right)$ (and analogously by $\ell_{+}\left(\mathcal{G}_{e v}(n, d)\right), \ell_{++}\left(\mathcal{G}_{e v}(n, d)\right)$ ). The subgroup $G_{e v}:=\left\{\pi s_{A} \mid A \in \mathcal{P}_{e v}\right\}$ of the group $G$ (introduced in (10)) acts vertex-transitively on $\mathcal{P}_{e v}$. Hence, applying Lemma $9, \ell\left(\mathcal{G}_{e v}(n, d)\right)$ can be formulated via the analogue of $(30)$, where $Y(y)$ in (31) is now indexed only by even sets; that is, $a, b, A$ and $B$ in (31) are indexed by $\mathcal{P}_{e v}$. Again, $A$ belongs to the Bose-Mesner algebra and $B$ belongs to the Terwilliger algebra; that is, for some scalars $x_{k}, x_{i, j}^{t}, A$ (resp., $B$ ) is equal to the principal submatrix of $\sum_{k \text { even }} x_{k} M_{k}$ (resp., of $\left.\sum_{i, j, t \text { even }} x_{i, j}^{t} M_{i, j}^{t}\right)$ indexed by $\mathcal{P}_{e v}$. Therefore, $\ell\left(\mathcal{G}_{e v}(n, d)\right)$ can be computed via the program:

$$
\begin{array}{ll}
\ell\left(\mathcal{G}_{e v}(n, d)\right)=\max 2^{n-1} x_{0,0}^{0} \quad \text { s.t. } \quad & x_{i, j}^{t}(i, j, t=0, \ldots, n) \text { satisfy }  \tag{55}\\
& (35),(36),(39)(i)-(i i i),(52)
\end{array}
$$

where, in (39), we consider only the 'even half of the matrices $A_{k}(x), B_{k}(x)$, i.e., their principal submatrices indexed by even indices $i, j$.
LEMMA 11. $A(n, d) \leq \ell\left(\mathcal{G}_{e v}(n, d)\right) \leq \ell^{0}(\mathcal{G}(n, d)) \leq \ell(\mathcal{G}(n, d))$ and analogously for the parameters $\ell_{+}, \ell_{\text {sch }}, \ell_{++}$.
Proof. The right and left most inequalities are obvious. To compare the parameters $\ell\left(\mathcal{G}_{e v}(n, d)\right)$ and $\ell^{0}(\mathcal{G}(n, d))$, it is easiest to use their formulation via (23); for the formulation of $\ell^{0}(\mathcal{G}(n, d))$, one should add to (23) the constraint (51) for any $\mathcal{A} \in \mathcal{P}_{3}(\mathcal{P})$. Consider a feasible solution $y$ for the program (23) defining $\ell\left(\mathcal{G}_{e v}(n, d)\right)$. Thus $y$ is indexed
by $\mathcal{P}_{3}\left(\mathcal{P}_{e v}\right), y_{\{I, J\}}=0$ if $|I \Delta J|=1, \ldots, d-1$ (for $I, J \in \mathcal{P}_{e v}$ ) and, for any $I \in \mathcal{P}_{e v}$, the matrix $Y_{I}(y)$ (indexed by $\mathcal{P}_{2}\left(\mathcal{P}_{e v} ; I\right)$ ) is positive semidefinite. We define a feasible solution $z$ for the program defining $\ell^{0}(\mathcal{G}(n, d))$ in the following way: For $\mathcal{A} \in \mathcal{P}_{3}(\mathcal{P})$, set $z_{\mathcal{A}}:=y_{\mathcal{A}}$ if $\mathcal{A} \subseteq \mathcal{P}_{e v}$, and $z_{\mathcal{A}}:=0$ otherwise. It is easy to verify that, for each $I \in \mathcal{P}$, the matrix $Y_{I}(z)$ (indexed by $\left.\mathcal{P}_{2}(\mathcal{P} ; I)\right)$ is positive semidefinite. Thus, $\ell^{0}(\mathcal{G}(n, d)) \geq \sum_{I \in \mathcal{P}} z_{I}=\sum_{I \in \mathcal{P}_{e v}} y_{I}$, implying $\ell^{0}(\mathcal{G}(n, d)) \geq \ell\left(\mathcal{G}_{e v}(n, d)\right)$. The reasoning is analogous for the other parameters.

The bound $\ell\left(\mathcal{G}_{e v}(n, d)\right)$ is more economical to compute than $\ell^{0}(\mathcal{G}(n, d))$, since it involves smaller matrices; as a matter of fact, the bound computed by Schrijver [13] is the bound $\ell_{s c h}\left(\mathcal{G}_{e v}(n, d)\right)$. For $n$ odd, in view of (53), all variables $z_{i, j}^{t}$ can be set to 0 for the computation of $\ell_{++}(\mathcal{G}(n, d))$; from this follows that $\ell_{+}\left(\mathcal{G}_{e v}(n, d)\right)=\ell_{++}\left(\mathcal{G}_{e v}(n, d)\right)$ when $n$ is odd.
3.3.5. Some computational results. We have tested the various bounds on several instances $(n, d)$, in particular, on those where Schrijver's bound gave a improvement on the previously best known upper bound for $A(n, d)$. There are two instances: $(20,8)$ and $(25,6)$, for which we could find an upper bound for $A(n, d)$ (slightly) better than Schrijver's bound; namely, $\left\lfloor\ell_{+}\left(\mathcal{G}_{e v}(25,6)\right)\right\rfloor$ and $\left\lfloor\ell_{++}\left(\mathcal{G}_{e v}(20,8)\right)\right\rfloor$ improve the upper bound given by Schrijver by one. See Table 1 below (the values given there are the bounds rounded down to the nearest integer). For other instances $(n, d)$, the bounds $\ell_{+}$and $\ell_{++}$give an improvement over Schrijver's bound limited to some decimals, thus yielding no improved upper bound on $A(n, d)$. Our computations were made using the NEOS Server for Optimization, which can be accessed at http://www-neos.mcs.anl.gov/, and we used specifically the software DSDP for semidefinite programming.

We indicate in Table 2 the sizes of the semidefinite programs involved in our computations. (In the 'block sizes' column in Table 2, $-N$ indicates that the last block is a diagonal matrix of order $N$.)

| $(n, d)$ | Delsarte <br> bound | Schrijver bound <br> $\ell_{\text {sch }}\left(\mathcal{G}_{e v}(n, d)\right)$ | $\ell_{+}\left(\mathcal{G}_{e v}(n, d)\right)$ | $\ell_{++}\left(\mathcal{G}_{e v}(n, d)\right)$ | $\ell_{+}^{0}(\mathcal{G}(n, d))$ | $\ell_{++}^{0}(\mathcal{G}(n, d))$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $(20,8)$ | 290 | 274 | 274 | 273 | 274 | 273 |
| $(25,6)$ | 48148 | 47998 | 47997 | 47997 | 47998 | 47998 |
| Table 1 |  |  |  |  |  |  |


| bound | $\#$ <br> var. | $\#$ <br> blocks | block sizes |
| :---: | :---: | :---: | :---: | :---: |
| $\ell_{+}\left(\mathcal{G}_{e v}(25,6)\right)$ | 131 | 27 | $1314121211111010998877665544332211-436$ |
| $\ell_{+}\left(\mathcal{G}_{e v}(20,8)\right)$ | 43 | 23 | 111299997777555533331111 -128 |
| $\ell_{++}\left(\mathcal{G}_{e v}(20,8)\right)$ | 68 | 12 | 342727212115159933 -221 |

Table 2: \# var. means 'number of variables', \# blocks means 'number of blocks'

De Klerk and Pasechnik [1] have recently applied the bound of Schrijver [13] and our bound $\ell_{+}$for finding tighter upper bounds for the stability number of the orthogonality graph $\Omega(n) ; \Omega(n)$ is the graph with node set $\mathcal{P}$, with an edge $(I, J)$ if $|I \Delta J|=n / 2$ (for $I, J \in \mathcal{P})$. Namely, to obtain an upper bound for the stability number of $\Omega(n)$, they propose to use the program (42) defining Schrijver's bound, or the program (41) defining the parameter $\ell_{+}$, replacing the constraint (36) by the constraint:

$$
x_{i, j}^{t}=0 \text { if }\{i, j, i+j-2 t\} \cap\{n / 2\} \neq \emptyset .
$$

The only interesting case is when $n$ is a multiple of 4 , since $\Omega(n)$ is the empty graph for $n$ odd and $\Omega(n)$ is a bipartite graph for $n=2 \bmod 4$. The computations made by de Klerk and Pasechnik [1], quoted in Table 3 below, indicate that the bound $\ell_{+}(\Omega(n))$ may give a much better upper bound for $\alpha(\Omega(n))$ than Schrijver's method. This contrasts with the situation encountered in the present paper, where the bound $\ell_{+}$gave only a moderate improvement upon Schrijver's bound for the instances of the coding problem we have tested.

| $n$ | $\ell_{+}(\Omega(n))$ | Schrijver's bound |
| :---: | :---: | :---: |
| 16 | 2304 | 2304 |
| 20 | $20,166.62$ | $20,166.98$ |
| 24 | 183,373 | 184,194 |
| 28 | $1,848,580$ | $1,883,009$ |
| 32 | $21,103,609$ | $21,723,404$ |

Table 3: [1] Comparing the bounds for the orthogonality graph $\Omega(n)$

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