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FULL LENGTH PAPER

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 et al. (Math Program, 2006) 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 (IEEE Trans. Inform. Theory 51:2859–2866, 2005) is located between the first and second bounds in the hierarchy. While computing the second bound involves a semidefinite program with $O(n^7)$ variables and thus seems out of reach for interesting values of n, Schrijver's bound can be computed via a semidefinite program of size $O(n^3)$, 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.

Keywords Stability number · Binary code · Semidefinite programming · Terwilliger algebra · Regular $*$-representation

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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

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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 $O(n^3)$ 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 $\vartheta(\mathcal{G})$, which can be computed, e.g., via the semidefinite program:

$$\begin{aligned}\vartheta(\mathcal{G}) := \max\ \textstyle\sum_{i\in\mathcal{V}} X_{ii}\ \text{ s.t. }\ & X = (X_{ij})_{i,j\in\mathcal{V}\cup\{0\}} \succeq 0,\ X_{00} = 1,\\ & X_{0i} = X_{ii}\ (i \in \mathcal{V}),\ X_{ij} = 0\ (ij \in \mathcal{E}).\end{aligned} \tag{1}$$

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 $\vartheta'(\mathcal{G})$ of $\vartheta(\mathcal{G})$ obtained by adding the nonnegativity constraint $X \geq 0$ to the program (1) and proved that $\vartheta'(\mathcal{G}(n,d))$ coincides with Delsarte bound.

Various methods have been proposed in the literature 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 kth iteration; see Sect. 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 Sect. 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 et al. [2], recalled in Sect. 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 $\vartheta'(\mathcal{G})$ 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 $O(n^3)$ 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 $O(n^7)$ variables.

In Sect. 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 $O(n^3)$. 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 $O(n^3)$ 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

$$\mathcal{P}_k(\mathcal{V}) := \{I \subseteq \mathcal{V} \mid |I| \leq k\} \text{ and } \mathcal{P}_{=k}(\mathcal{V}) := \{I \subseteq \mathcal{V} \mid |I| = k\}.$$

We let $Sym(\mathcal{V})$ denote the set of all permutations of the set $\mathcal{V}$ and we set $Sym(n) := Sym(\mathcal{V})$ 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 $h : G \to Sym(\mathcal{X})$, where $Sym(\mathcal{X})$ is the group of permutations of $\mathcal{X}$. For $\sigma \in G$, $h(\sigma)$ is a permutation of $\mathcal{X}$ and M_σ is the associated $\mathcal{X} \times \mathcal{X}$ permutation matrix with

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

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

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

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

$$\mathcal{A}^G := \{N \in \mathbb{C}^{\mathcal{X} \times \mathcal{X}} \mid NM = MN\ \forall M \in \mathcal{A}\},$$

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 the 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:

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

Then, $\tilde{D}_1, \ldots, \tilde{D}_N$ form a basis of the commutant $\mathcal{A}^G$ (as vector space) and $\tilde{D}_1 + \cdots + \tilde{D}_N = J$ (the all-ones matrix). We normalize the $\tilde{D}_i$ to

$$D_i := \frac{\tilde{D}_i}{\sqrt{\langle \tilde{D}_i, \tilde{D}_i \rangle}} \tag{3}$$

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

$$D_i D_j = \sum_{k=1}^N \gamma_{i,j}^k D_k \tag{4}$$

for all $i, j = 1, \ldots, N$. Define the $N \times N$ matrices $L_1, \ldots, L_N$ by

$$(L_k)_{i,j} := \gamma_{k,j}^i \quad \text{for } k, i, j = 1, \ldots, N. \tag{5}$$

De Klerk et al. [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 $x_1, \ldots, x_N$,*

$$\sum_{i=1}^{N} x_i D_i \succeq 0 \Longleftrightarrow \sum_{i=1}^{N} x_i L_i \succeq 0. \tag{6}$$

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

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

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 $\ell' \in \{1, \ldots, m\}$ such that $\sigma(A_\ell) = A_{\ell'}$ and $b_\ell = b_{\ell'}$.) 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 1 *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*

$$\min \sum_{i=1}^{N} c_i x_i \ \ s.t. \ a_\ell^{\mathrm{T}} x \leq b_\ell \ (\ell = 1, \ldots, m), \quad \sum_{i=1}^{N} x_i L_i \succeq 0. \tag{8}$$

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 et al. [2] apply this technique for computing tighter bounds for the crossing number of a complete bipartite graph. We apply it in Sect. 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 1 Let $\mathcal{X} := \mathcal{P}$, the collection of all subsets of the set $V = \{1, \ldots, n\}$, and $G := Sym(V)$, the group of permutations of V. Each $\pi \in G$ induces a permutation of $\mathcal{X}$, again denoted by π, by letting $\pi(I) := \{\pi(i) \mid i \in I\}$ for $I \in \mathcal{P}$. Two pairs $(I,J),(I',J')$ $(I,J,I',J' \in \mathcal{P})$ lie in the same orbit [i.e., $I' = \pi(I)$, $J' = \pi(J)$ for some $\pi \in G$] if and only if $|I| = |I'|$, $|J| = |J'|$ and $|I \cap J| = |I' \cap J'|$. Therefore, the commutant algebra $\mathcal{A}^G$ is generated by the matrices $M^t_{i,j}$ $(i,j,t \in \mathbb{Z}_+)$, where

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

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

Example 2 Consider again the set $\mathcal{X} := \mathcal{P}$, but now the group is $G := Aut(\mathcal{P})$, the automorphism group of $\mathcal{P}$. The group G consists of the permutations $\sigma \in Sym(\mathcal{P})$ preserving the symmetric difference, i.e., for which $|\sigma(I)\Delta\sigma(J)| = |I\Delta J|$ for all $I,J \in \mathcal{P}$. Thus,

$$G = \{\pi s_A \mid A \subseteq V, \pi \in Sym(V)\} \tag{10}$$

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 $(I,J),(I',J')$ $(I,J,I',J' \in \mathcal{P})$ lie in the same orbit [i.e., $I' = \sigma(I)$, $J' = \sigma(J)$ for some $\sigma \in G$] if and only if $|I\Delta J| = |I'\Delta J'|$. Therefore, the algebra $\mathcal{A}^G$ is generated by the matrices M_k $(k = 0,1,\ldots,n)$ where

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

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 $\dim \mathcal{A}_n = \binom{n+3}{3}$, 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 $U^*\mathcal{A}_nU := \{U^*MU \mid M \in \mathcal{A}_n\}$ is equal to the collection of block-diagonal matrices

$$\begin{pmatrix} C_0 & 0 & \ldots & 0 \\ 0 & C_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \ldots & C_m \end{pmatrix},$$

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:

$$C_k = \begin{pmatrix} B_k & 0 & \ldots & 0 \\ 0 & B_k & \ldots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \ldots & B_k \end{pmatrix};$$

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

$$\bigoplus_{k=0}^{m} \mathbb{C}^{p_k \times p_k} = \left\{ \begin{pmatrix} B_0 & 0 & \ldots & 0 \\ 0 & B_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \ldots & B_m \end{pmatrix} \mid B_k \in \mathbb{C}^{p_k \times p_k} \text{ for } k = 0, 1, \ldots, m \right\}. \quad (12)$$

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, $m = \lfloor \frac{n}{2} \rfloor$ and, for $k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$, the block B_k has order $p_k = n - 2k + 1$ 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 $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, define

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

Let $\mathcal{B}_k$ be a basis of $\mathcal{L}_k$. Then $|\mathcal{B}_k| = \binom{n}{k} - \binom{n}{k-1}$ and $\sum_{I\in\mathcal{P}} b_I = 0$ for $b \in \mathcal{L}_k$. Set $\mathcal{B}_0 := \{b_0\}$ where $b_0 := (1, 0, \ldots, 0)^{\mathrm{T}} \in \mathbb{R}^{\mathcal{P}}$ (the nonzero entry being indexed by $\emptyset \in \mathcal{P}$) and define

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

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

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

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 1 [13] *The matrix U is orthogonal, i.e., $U^{\mathrm{T}}U = I$. Moreover, for a matrix $M = \sum_{i,j,t=0}^n x^t_{i,j} M^t_{i,j} \in \mathcal{A}_n$ (with $x^t_{i,j} \in \mathbb{R}$), the matrix $U^{\mathrm{T}}MU$ is a block-diagonal matrix determined by the partition of $\mathcal{Q}$ into the classes $\mathcal{Q}_{k,b} := \{(k, i, b) \mid k \le i \le n-k\}$ (for $k = 0, \ldots, \lfloor\frac{n}{2}\rfloor$, $b \in \mathcal{B}_k$). For a given integer $k = 0, \ldots, \lfloor\frac{n}{2}\rfloor$, the blocks corresponding to the classes $\mathcal{Q}_{k,b}$ (for $b \in \mathcal{B}_k$) are all identical to the following matrix:*

$$B_k(x) := \left(\sum_t \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}} \beta^t_{i,j,k} x^t_{i,j}\right)_{i,j=k}^{n-k}, \tag{13}$$

after setting

$$\beta^t_{i,j,k} := \sum_{u=0}^n (-1)^{t-u} \binom{u}{t} \binom{n-2k}{n-k-u} \binom{n-k-u}{i-u} \binom{n-k-u}{j-u} \tag{14}$$

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

$$\sum_{i,j,t=0}^n x^t_{i,j} M^t_{i,j} \succeq 0 \iff B_k(x) \succeq 0 \quad \text{for } k = 0, 1, \ldots, \lfloor\frac{n}{2}\rfloor. \tag{15}$$

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 $O(n^3)$.

We will deal in this paper with matrices of the form

$$\tilde{M} = \begin{pmatrix} d & c^{\mathrm{T}} \\ c & M \end{pmatrix}, \quad \text{where } M = \sum_{i,j,t=0}^n x^t_{i,j} M^t_{i,j}, \quad d \in \mathbb{R}, \quad c = \sum_{i=0}^n c_i \chi^{\mathcal{P}_{=i}(V)}. \tag{16}$$

Recall that $\mathcal{P}_{=i}(V) = \{I \subseteq V \mid |I| = i\}$ and $\chi^{\mathcal{P}_{=i}(V)} \in \{0,1\}^{\mathcal{P}}$ whose Ith entry is 1 if and only if $I \in \mathcal{P}_{=i}(V)$.

Lemma 1 *The matrix $\tilde{M}$ from (16) is positive semidefinite if and only if $B_k(x) \succeq 0$ for $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, and*

$$\tilde{B}_0(x) := \begin{pmatrix} d & \tilde{c}^{\mathrm{T}} \\ \tilde{c} & B_0(x) \end{pmatrix} \succeq 0, \quad \textit{where } \tilde{c} := \left(c_i \binom{n}{i}^{\frac{1}{2}} \right)_{i=0}^{n}.$$

Proof Setting

$$\tilde{U} := \begin{pmatrix} 1 & 0 \\ 0 & U^{\mathrm{T}} \end{pmatrix},$$

we have:

$$\tilde{U}^T \tilde{M} \tilde{U} = \begin{pmatrix} d & c^{\mathrm{T}} U \\ U^{\mathrm{T}} c & U^{\mathrm{T}} M U \end{pmatrix}.$$

It suffices now to verify that $(c^{\mathrm{T}} U)_{k,i,b} = c^{\mathrm{T}} u_{k,i,b} = 0$ for $(k, i, b) \in \mathcal{Q}$ with $k \geq 1$, and that $(c^{\mathrm{T}} U)_{0,i,b_0} = c_i \binom{n}{i}^{\frac{1}{2}}$ for $i = 0, \ldots, n$. This is direct verification using the above definitions; details are omitted. Hence, $\tilde{U}^{\mathrm{T}} \tilde{M} \tilde{U}$ is block-diagonal, with blocks $\tilde{B}_0(x)$ (with multiplicity 1) and $B_k(x)$ (with multiplicity q_k) for $k = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. 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 $\mathcal{P}_k(\mathcal{V}) = \{I \subseteq \mathcal{V} \mid |I| \leq k\}$ for an integer k. Given a stable set S in $\mathcal{G}$, define $x = (x_I)_{I \in \mathcal{P}_k(\mathcal{V})} \in \{0,1\}^{\mathcal{P}_k(\mathcal{V})}$ and $y = (y_I)_{I \in \mathcal{P}_{2k}(\mathcal{V})} \in \{0,1\}^{\mathcal{P}_{2k}(\mathcal{V})}$ 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 $I \in \mathcal{P}_{2k}(\mathcal{V})$). Then y and the matrix $Y := xx^T$ satisfy:

$$Y \succeq 0 \tag{17}$$

$$Y_{I,J} = y_{I \cup J} \ \ (\text{for } I, J \in \mathcal{P}_k(\mathcal{V})) \tag{18}$$

$$Y_{I,J} = y_{I \cup J} = 0 \ \text{ if } I \cup J \text{ contains an edge } \ (\text{for } I, J \in \mathcal{P}_k(\mathcal{V})) \tag{19}$$

$$Y_{\emptyset,\emptyset} = y_{\emptyset} = 1 \tag{20}$$

$$0 \leq y_I \leq y_J \ \text{ if } J \subseteq I \ (\text{for } I, J \in \mathcal{P}_{2k}(\mathcal{V})). \tag{21}$$

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 [6–8]). Under the assumption (17), the edge condition (19) is, in fact, equivalent to $y_{ij} = 0$ (for $ij \in \mathcal{E}$). (Here and below, we set $y_{ij} := y_{\{i\},\{j\}}$, $y_i := y_{\{i\}}$, 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 $\begin{pmatrix} y_I & y_J \\ y_J & y_J \end{pmatrix}$, whose positive semidefiniteness implies $0 \le y_J \le y_I$. On the other hand, $M_1(y) \succeq 0$ implies $|y_{ij}| \le \max(y_i, y_j)$; indeed the principal submatrix of $M_1(y)$ indexed by $\{\{i\}, \{j\}\}$ has the form $\begin{pmatrix} y_i & y_{ij} \\ y_{ij} & y_j \end{pmatrix}$, whose positive semidefiniteness implies $y_{ij}^2 \le y_i y_j \le \max(y_i^2, y_j^2)$. Similarly, $M_2(y) \succeq 0$ implies that $|y_{ijk}|$ is at most the largest two values among y_{ij}, y_{ik}, y_{jk}; indeed the principal submatrix of $M_2(y)$ indexed by the set $\{\{i,j\}, \{i,k\}, \{j,k\}\}$ has the form $\begin{pmatrix} y_{ij} & y_{ijk} & y_{ijk} \\ y_{ijk} & y_{ik} & y_{ijk} \\ y_{ijk} & y_{ijk} & y_{jk} \end{pmatrix}$, whose positive semidefiniteness implies $y_{ijk}^2 \le \min(y_{ij}y_{ik}, y_{ij}y_{jk}, y_{ik}y_{jk}) \le y_{ik}^2, y_{jk}^2$ assuming, say, that $y_{ij} \le y_{ik} \le y_{jk}$.

Consider the semidefinite program:

$$\ell^{(k)}(\mathcal{G}) := \max \sum_{i \in \mathcal{V}} y_i \text{ s.t. } M_k(y) \succeq 0, \quad y_\emptyset = 1, \quad y_{ij} = 0 \ (ij \in \mathcal{E}). \tag{22}$$

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

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

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 $\vartheta'(\mathcal{G})$, the strengthening of $\vartheta(\mathcal{G})$ introduced by McEliece et al. [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 $\mathrm{TH}(\mathcal{G})$ ([8]; or see (26)). For $k = 2$, the program (22) has size $O(|\mathcal{V}|^4)$. 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 $O(|\mathcal{V}|^3)$.

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

$$\ell(\mathcal{G}) := \max \sum_{i \in \mathcal{V}} y_i \text{ s.t. } y_\emptyset = 1, \quad y_{ij} = 0 \ (ij \in \mathcal{E}), \quad Y_r(y) \succeq 0 \ (r \in \mathcal{V}) \tag{23}$$

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

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

analogously for the ℓ_+ parameters. We will see in Sect. 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 $O(n^3)$.

From the moment condition (18), the matrix $Y_r(y)$ has the block structure:

$$Y_r(y) = \begin{pmatrix} 1 & a^{\mathrm{T}} & b_r^{\mathrm{T}} \\ a & A & B_r \\ b_r & B_r & B_r \end{pmatrix}, \tag{24}$$

where $A := (y_{ij})_{i,j\in\mathcal{V}}$, $B_r := (y_{\{i,j,r\}})_{i,j\in\mathcal{V}}$ are symmetric $\mathcal{V}\times\mathcal{V}$ matrices, and $a := (y_i)_{i\in\mathcal{V}}$, $b_r := (y_{ir})_{i\in\mathcal{V}}$. 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

$$Y_r(y) \succeq 0 \Longleftrightarrow B_r \succeq 0 \quad \text{and} \quad \tilde{C}_r := \begin{pmatrix} 1-y_r & a^{\mathrm{T}}-b_r^{\mathrm{T}} \\ a-b_r & A-B_r \end{pmatrix} \succeq 0, \tag{25}$$

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

$$\begin{aligned} \mathrm{TH}(\mathcal{G}) = \{x \in \mathbb{R}^{\mathcal{P}_1(\mathcal{V})} \mid \exists y \in \mathbb{R}^{\mathcal{P}_2(\mathcal{V})} \text{ s.t. } & M_1(y) \succeq 0,\ y_{ij} = 0\ (ij \in \mathcal{E}), \\ & x_I = y_I\ (I \in \mathcal{P}_1(\mathcal{V}))\}, \end{aligned}$$

$$\begin{aligned} N_+(\mathrm{TH}(\mathcal{G})) = \{x \in \mathbb{R}^{\mathcal{V}} \mid \exists y \in \mathbb{R}^{\mathcal{P}_2(\mathcal{V})} \text{ s.t. } & M_1(y) \succeq 0,\ y_\emptyset = 1,\ x_i = y_i\ (i \in \mathcal{V}), \\ & (y_{I\cup\{r\}})_{I\in\mathcal{P}_1(\mathcal{V})}, (y_I - y_{I\cup\{r\}})_{I\in\mathcal{P}_1(\mathcal{V})} \in \mathrm{TH}(\mathcal{G})\} \end{aligned}$$

one can verify that

$$\ell(\mathcal{G}) \le \max_{x\in N_+(\mathrm{TH}(\mathcal{G}))} \sum_{i\in\mathcal{V}} x_i. \tag{26}$$

To see it, let y be feasible for (23); then $x := (y_i)_{i\in\mathcal{V}} \in N_+(\mathrm{TH}(\mathcal{G}))$. Indeed, the vector $(y_{I\cup\{r\}})_{I\in\mathcal{P}_1(V)}$ 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 $(y_I - y_{I\cup\{r\}})_{I\in\mathcal{P}_1(V)}$ 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, $G \subseteq Sym(\mathcal{V})$ and each $\sigma \in G$ preserves edges, i.e., $ij \in \mathcal{E} \Longrightarrow \sigma(i)\sigma(j) \in \mathcal{E}$. 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 2 *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 ij 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 1, 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 $G = Aut(\mathcal{P})$, 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 $\{1,\dots,n\}$, with an edge (I,J) if $|I\Delta J| \in \{1,\dots,d-1\}$ for $I,J \in \mathcal{P}$. Thus G also acts on the set $\mathcal{P}_k(\mathcal{P}) = \{\mathcal{A} \subseteq \mathcal{P} \mid |\mathcal{A}| \le k\}$, indexing the matrix variable in program (22). We show:

Theorem 2 *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 2, 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 $r + s \ge 1$. Let $\vec{\mathcal{A}} = (A_1,\dots,A_r)$ be an ordering of the elements of $\mathcal{A}$; similarly, $\vec{\mathcal{B}} = (B_1,\dots,B_s)$ is an ordering of the elements of $\mathcal{B}$. Then one can define the $(r+s)\times n$ *incidence tableau* of $(\vec{\mathcal{A}},\vec{\mathcal{B}})$, whose rows are the incidence vectors $\chi^{A_1},\dots,\chi^{A_r},\chi^{B_1},\dots,\chi^{B_s}$ (in that order) of the sets $A_1,\dots,A_r,B_1,\dots,B_s$. Define the function $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}}: \{0,1\}^r \times \{0,1\}^s \longrightarrow \mathbb{Z}_+$ where, for $(u,v) \in \{0,1\}^r \times \{0,1\}^s$, $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}}(u,v)$ is the multiplicity of (u,v) as a column of the incidence tableau of $(\vec{\mathcal{A}},\vec{\mathcal{B}})$. Thus $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}}$ belongs to the set $\Phi_{r,s}$ consisting of the functions $\phi : \{0,1\}^r \times \{0,1\}^s \longrightarrow \{0,1,\dots,n\}$ satisfying: $\sum_{u\in\{0,1\}^r, v\in\{0,1\}^s}$

$\phi(u, v) = n$ and, for all $i \neq j \in \{1, \dots, r\}$ (resp., $i \neq j \in \{1, \dots, s\}$), there exists $(u, v) \in \{0, 1\}^r \times \{0, 1\}^s$ for which $\phi(u, v) \geq 1$ and $u_i \neq u_j$ (resp., $v_i \neq v_j$).

Let $\vec{\mathcal{A}}'$ (resp., $\vec{\mathcal{B}}'$) be another ordered sequence of r (resp., of s) distinct elements of $\mathcal{P}$ and let $\phi = \phi_{\vec{\mathcal{A}},\vec{\mathcal{B}}}$, $\phi' = \varphi_{\vec{\mathcal{A}}',\vec{\mathcal{B}}'}$. Then, $\vec{\mathcal{A}}' = (\sigma(A_1), \dots, \sigma(A_r))$ and $\vec{\mathcal{B}}' = (\sigma(B_1), \dots, \sigma(B_s))$ for some $\sigma \in G$ if and only if $\phi(u, v) + \phi(\mathbf{1} - u, \mathbf{1} - v) = \phi'(u, v) + \phi'(\mathbf{1} - u, \mathbf{1} - v)$ for all $(u, v) \in \{0, 1\}^r \times \{0, 1\}^s$. (Here, $\mathbf{1} := (1, \dots, 1)$ denotes the all-ones vector of the suitable size.) Moreover, $\vec{\mathcal{A}}' = (A_{\alpha(1)}, \dots, A_{\alpha(r)})$ and $\vec{\mathcal{B}}' = (B_{\beta(1)}, \dots, B_{\beta(s)})$ for some permutations $\alpha \in Sym(r)$, $\beta \in Sym(s)$ if and only if $\phi'(u, v) = \phi(\alpha(u), \beta(v))$ for all $(u, v) \in \{0, 1\}^r \times \{0, 1\}^s$, setting $\alpha(u) := (u_{\alpha(1)}, \dots, u_{\alpha(r)}), \beta(v) := (v_{\beta(1)}, \dots, v_{\beta(s)})$. For two elements $\phi, \phi' \in \Phi_{r,s}$, write $\phi \sim \phi'$ if there exist $\alpha \in Sym(r)$, $\beta \in Sym(s)$ for which

$$\phi'(u, v) + \phi'(\mathbf{1} - u, \mathbf{1} - v) = \phi(\alpha(u), \beta(v)) + \phi(\mathbf{1} - \alpha(u), \mathbf{1} - \beta(v)))$$
$$\text{for all } (u, v) \in \{0, 1\}^r \times \{0, 1\}^s.$$

This defines an equivalence relation on $\Phi_{r,s}$.

We can now characterize orbits in the following way: Two pairs $(\mathcal{A}, \mathcal{B})$ and $(\mathcal{A}', \mathcal{B}')$ 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 $|\mathcal{A}| = |\mathcal{A}'| =: r$, $|\mathcal{B}| = |\mathcal{B}'| =: s$ and $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}} \sim \varphi_{\vec{\mathcal{A}}',\vec{\mathcal{B}}'}$ for some respective orderings $\vec{\mathcal{A}}$, $\vec{\mathcal{B}}$, $\vec{\mathcal{A}}'$, $\vec{\mathcal{B}}'$ of $\mathcal{A}$, $\mathcal{B}$, $\mathcal{A}'$, $\mathcal{B}'$. 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 $1 + \sum_{\substack{0 \leq r,s \leq k \\ r+s \geq 1}} (n+1)^{2^{r+s-1}-1}$, giving:

$$N_k \leq O(n^{2^{2k-1}-1}). \tag{27}$$

We now verify that the matrices L_i ($i = 1, \dots, N_k$) (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_{ϕ_0} of pairs $(\mathcal{A}, \mathcal{B}) \in \mathcal{P}_{=r}(\mathcal{P}) \times \mathcal{P}_{=s}(\mathcal{P})$ for which $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}} \sim \phi_0$ for some orderings $\vec{\mathcal{A}}$, $\vec{\mathcal{B}}$ 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 $(\vec{\mathcal{A}}, \vec{\mathcal{B}})$ for which $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}} = \phi_0$. 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 ϕ_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 $\vec{\mathcal{A}}$, $\vec{\mathcal{B}}$, 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_{ϕ_0,ψ_0} of elements $\mathcal{C} \in \mathcal{P}_{=t}(\mathcal{P})$ for which $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{C}}} \sim \phi_0$ and $\varphi_{\vec{\mathcal{B}},\vec{\mathcal{C}}} \sim \psi_0$ for some ordering $\vec{\mathcal{C}}$ of $\mathcal{C}$. Set $\xi := \varphi_{\vec{\mathcal{A}},\vec{\mathcal{B}}}$. Given $\phi \sim \phi_0$ and $\psi \sim \psi_0$, we first count the number $\ell_{\phi,\psi}$ of ordered sequences $\vec{\mathcal{C}}$ of t elements of $\mathcal{P}$ for which $\varphi_{\vec{\mathcal{A}},\vec{\mathcal{C}}} = \phi$ and $\varphi_{\vec{\mathcal{B}},\vec{\mathcal{C}}} = \psi$. For this let $x(u, v, w)$ denote the multiplicity of $(u, v, w) \in \{0, 1\}^r \times \{0, 1\}^s \times \{0, 1\}^t$ as column of the incidence tableau of $(\vec{\mathcal{A}}, \vec{\mathcal{B}}, \vec{\mathcal{C}})$. 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

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

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, $\ell_{\phi,\psi} = \sum_{x\in S} \sum_{u\in\{0,1\}^r, v\in\{0,1\}^s} \frac{\xi(u,v)!}{\prod_{w\in\{0,1\}^t} x(u,v,w)!}$, the number of possible ways to assign the vectors $w \in \{0,1\}^t$ as columns of the lower $t \times n$ part of the tableau. Now, $L_{\phi_0,\psi_0} = \frac{1}{t!} \sum_{\substack{\phi\sim\phi_0 \\ \psi\sim\psi_0}} \ell_{\phi,\psi}$ can be computed in time polynomial in n since one can enumerate the equivalence classes of ϕ_0 and ψ_0.

Remains only to construct the linear constraints corresponding to the moment constraints (18) and the edge constraints (19). Label the orbits of the set $\mathcal{P}_k(\mathcal{P}) \times \mathcal{P}_k(\mathcal{P})$ as $\mathcal{O}_1, \ldots, \mathcal{O}_{N_k}$ and determine a pair $(\mathcal{A}_i, \mathcal{B}_i)$ belonging to each orbit $\mathcal{O}_i$. Then the moment constraints read: $x_i = x_j$ if $\mathcal{A}_i \cup \mathcal{B}_i = \sigma(\mathcal{A}_j \cup \mathcal{B}_j)$ 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: $x_i \geq 0$ $(i = 1,\ldots,N_k)$ and $x_i \leq x_j$ if $\mathcal{A}_i \cup \mathcal{B}_i \supseteq \sigma(\mathcal{A}_j \cup \mathcal{B}_j)$ for some $\sigma \in G$ (which can be tested in time polynomial in n).

Therefore, the parameter $\ell^{(k)}(\mathcal{G}(n,d))$ (or $\ell_+^{(k)}(\mathcal{G}(n,d))$) 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 $O(N_k^2)$ linear constraints. As $N_k = O(n^{2^{2k-1}-1})$, it can be computed in time polynomial in n (to any precision), which concludes the proof of Theorem 2. □

The result from Theorem 2 is mainly of theoretical value for $k \geq 2$. Indeed, for $k=2$, $N_k = O(n^7)$ 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 3 *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 2. Here, we use the fact that, for $r \in \mathcal{V}$, $\sigma \in G$, $Y_r(\sigma(y)) = \sigma(Y_{\sigma(r)}(y))$. 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 $G = Aut(\mathcal{P})$, whose action on the graph $\mathcal{G}(n,d)$ is indeed vertex-transitive. We set:

$$\mathcal{X} := \mathcal{P}_2(\mathcal{P};\emptyset) = \{\emptyset\} \cup \{\{I\} \mid I \in \mathcal{P}\} \cup \{\{\emptyset, I\} \mid I \in \mathcal{P}\}. \tag{29}$$

Applying Lemma 3, one can reformulate the parameter $\ell(\mathcal{G}(n,d))$ as

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

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

$$Y(y) = \begin{pmatrix} 1 & a^{\mathrm{T}} & b^{\mathrm{T}} \\ a & A & B \\ b & B & B \end{pmatrix} \tag{31}$$

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

$$A = \sum_{k=0}^{n} x_k M_k \text{ for some real scalars } x_0,\ldots,x_n, \tag{32}$$

where the matrices M_k are as in (11). Moreover, $B_{I,J} = B_{I',J'}$ if $I' = \sigma(I)$, $J' = \sigma(J), \emptyset = \sigma(\emptyset)$ for some $\sigma \in G$, i.e., if $|I'| = |I|, |J'| = |J|$ and $|I\cap J| = |I'\cap J'|$. That is, the matrix B belongs to the Terwilliger algebra $\mathcal{A}_n$; say,

$$B = \sum_{i,j,t\geq 0} x^t_{i,j} M^t_{i,j} \text{ for some real scalars } x^t_{i,j}, \tag{33}$$

where the matrices $M^t_{i,j}$ are as in (9) and $x^t_{i,j} = x^t_{j,i}$ for all i,j,t. The variables x_k and $x^t_{i,j}$ are related by

$$x_k = x^0_{0,k} \quad \text{for } k = 0,1,\ldots,n \tag{34}$$

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

$$x^t_{i,j} = x^{t'}_{i',j'} \text{ if } (i', j', i' + j' - 2t') \text{ is a permutation of } (i, j, i + j - 2t). \tag{35}$$

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

$$x^t_{i,j} = 0 \text{ if } \{i, j, i + j - 2t\} \cap \{1, \ldots, d - 1\} \neq \emptyset, \tag{36}$$

and the bounds (21) read:

$$0 \le x^t_{i,j} \le x^0_{i,0} \quad \text{for } i, j, t = 0, \ldots, n. \tag{37}$$

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

$$B = \sum_{i,j,t=0}^{n} x^t_{i,j} M^t_{i,j} \succeq 0 \quad \text{and} \quad \tilde{C} := \begin{pmatrix} 1 - x^0_{0,0} & c^{\mathrm{T}} \\ c & C \end{pmatrix} \succeq 0,$$

where

$$C := A - B = \sum_{i,j,t=0}^{n} (x^0_{0,i+j-2t} - x^t_{i,j}) M^t_{i,j} \quad \text{and} \quad c := a - b = \sum_{i=0}^{n} (x^0_{0,0} - x^0_{0,i}) \chi^{\mathcal{P}_{=i}(V)}.$$

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

$$A_k(x) := \left(\sum_t \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}} \beta^t_{i,j,k} x^0_{0,i+j-2t} \right)_{i,j=k}^{n-k} \tag{38}$$

and $B_k(x)$ as in (13), where $\beta^t_{i,j,k}$ are as in (14). It follows from Lemma 1 that the positive semidefiniteness of $Y(y)$ is equivalent to

$$\begin{array}{l} \text{(i) } B_k(x) \succeq 0 \text{ for } k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor \\ \text{(ii) } A_k(x) - B_k(x) \succeq 0 \text{ for } k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor \\ \text{(iii)} \begin{pmatrix} 1 - x^0_{0,0} & \tilde{c}^T \\ \tilde{c} & A_0(x) - B_0(x) \end{pmatrix} \succeq 0, \text{ setting } \tilde{c} := (\binom{n}{i}^{\frac{1}{2}} (x^0_{0,0} - x^0_{0,i}))^n_{i=0}. \end{array} \tag{39}$$

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

$$\ell(\mathcal{G}(n,d)) = \max \ 2^n x^0_{0,0} \ \text{s.t.} \ x^t_{i,j} \ (i, j, t = 0, \ldots, n) \text{ satisfy } (35), (36), (39)(i) - (iii). \tag{40}$$

Similarly,

$$\ell_+(\mathcal{G}(n,d)) = \max\ 2^n x^0_{0,0} \ \text{ s.t. } \ x^t_{i,j}\ (i,j,t=0,\ldots,n) \text{ satisfy } (35),(36),(37),(39)(i)\text{–}(iii). \tag{41}$$

Hence both parameters can be computed via a semidefinite program of size $O(n^3)$.

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 $\mathcal{G}(n,d)$:

$$\begin{aligned} \ell_{sch}(\mathcal{G}(n,d)) := \max \sum_{i=0}^{n} \binom{n}{i} x^0_{0,i} \\ \text{s.t. } x^t_{i,j}\ (i,j,t=0,\ldots,n) \ \text{ satisfy } (35),(36),(37), \\ (39)(i)-(ii), \text{ and } x^0_{0,0}=1. \end{aligned} \tag{42}$$

As noted in [13], Schrijver's bound is at least as good as the Delsarte bound, which coincides with $\vartheta'(\mathcal{G}(n,d)) = \ell^{(1)}_+(\mathcal{G}(n,d))$. We now show:

Lemma 4 *The bound $\ell_+(\mathcal{G}(n,d))$ from (41) is at least as good as Schrijver's bound $\ell_{sch}(\mathcal{G}(n,d))$ from (42); that is, $\ell_+(\mathcal{G}(n,d)) \le \ell_{sch}(\mathcal{G}(n,d))$.*

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

$$\begin{pmatrix} 1 & a^{\mathrm{T}} \\ a & A \end{pmatrix} \succeq 0, \ \text{ i.e., } A - aa^{\mathrm{T}} \succeq 0,$$

where A is as in (32), $a^{\mathrm{T}} = (x^0_{0,0},\ldots,x^0_{0,0})$, $x_k = x^0_{0,k}$ for $k=0,\ldots,n$. Thus, $aa^{\mathrm{T}} = (x^0_{0,0})^2 J$, where J is the all-ones matrix. As $A-(x^0_{0,0})^2 J \succeq 0$, we deduce that $\langle J,A\rangle \ge (x^0_{0,0})^2\langle J,J\rangle = (x^0_{0,0}2^n)^2$. But $\langle J,A\rangle = \sum_{k=0}^n x_k\langle J,M_k\rangle = \sum_{k=0}^n x_k 2^n\binom{n}{k}$, which gives $\sum_{k=0}^n x^0_{0,k}\binom{n}{k} \ge 2^n (x^0_{0,0})^2$. □

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

$O(n^3)$. Namely, let us now consider as matrix variable the principal submatrix $Y(y)$ of $M_2(y)$ indexed by the set

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

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

$$Y(y) = \begin{pmatrix} 1 & a^{\mathrm{T}} & b^{\mathrm{T}} & c^{\mathrm{T}} \\ a & A & B & C \\ b & B & B & D \\ c & C & D & C \end{pmatrix}, \tag{44}$$

where $A = (y_{\{I,J\}})_{I,J\in\mathcal{P}}, B = (y_{\{\emptyset,I,J\}})_{I,J\in\mathcal{P}}, C = (y_{\{I,J,V\}})_{I,J\in\mathcal{P}}$, $D = (y_{\{\emptyset,I,J,V\}})_{I,J\in\mathcal{P}}$, $a = (y_{\{I\}})_{I\in\mathcal{P}}, b = (y_{\{\emptyset,I\}})_{I\in\mathcal{P}}$, and $c = (y_{\{I,V\}})_{I\in\mathcal{P}}$. 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, $D_{I,J} = D_{I',J'}$ if there exists $\sigma \in G$ such that $\sigma(\emptyset) = \emptyset$, $\sigma(I) = I', \sigma(J) = J'$ (then $\sigma(V) = V$), i.e., if $|I| = |I'|, |J| = |J'|, |I \cap J| = |I' \cap J'|$. We have the following relations for the variables $x_{i,j}^t$, $z_{i,j}^t$:

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

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

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

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:

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

The bounds (21) imply:

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

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & U^{\mathrm{T}} & 0 & 0 \\ 0 & 0 & U^{\mathrm{T}} & 0 \\ 0 & 0 & 0 & U^{\mathrm{T}} \end{pmatrix} Y(y) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & U & 0 & 0 \\ 0 & 0 & U & 0 \\ 0 & 0 & 0 & U \end{pmatrix} = \begin{pmatrix} 1 & a^{\mathrm{T}}U & b^{\mathrm{T}}U & c^{\mathrm{T}}U \\ Ua & U^{\mathrm{T}}AU & U^{\mathrm{T}}BU & U^{\mathrm{T}}CU \\ Ub & U^{\mathrm{T}}BU & U^{\mathrm{T}}BU & U^{\mathrm{T}}DU \\ Uc & U^{\mathrm{T}}CU & U^{\mathrm{T}}DU & U^{\mathrm{T}}CU \end{pmatrix}$$

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

$$\begin{pmatrix} 1 & \tilde{a}^{\mathrm{T}} & \tilde{b}^{\mathrm{T}} & \tilde{c}^{\mathrm{T}} \\ \tilde{a} & A_0 & B_0 & C_0 \\ \tilde{b} & B_0 & B_0 & D_0 \\ \tilde{c} & C_0 & D_0 & C_0 \end{pmatrix} \succeq 0, \quad \begin{pmatrix} A_k & B_k & C_k \\ B_k & B_k & D_k \\ C_k & D_k & C_k \end{pmatrix} \succeq 0 \quad \text{for } k = 1, \ldots, \lfloor \frac{n}{2} \rfloor, \tag{49}$$

where $A_k = A_k(x)$ is as in (38), $B_k = B_k(x)$ is as in (13) and

$$C_k = \left(\sum_t \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}} \beta^t_{i,j,k} x^{n+t-i-j}_{n-i,n-j} \right)_{i,j=k}^{n-k},$$

$$D_k = \left(\sum_t \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}} \beta^t_{i,j,k} z^t_{i,j} \right)_{i,j=k}^{n-k}.$$

One can now define the bound

$$\ell_{++}(\mathcal{G}(n,d)) := \max 2^n x^0_{0,0} \ \text{ s.t. } x^t_{i,j},\ z^t_{i,j}\ (i,j,t = 0, \ldots, n) \text{ satisfy} \\ (35), (36), (37), (45), (46), (47), (48) \text{ and } (49). \tag{50}$$

Obviously,

$$A(n,d) \leq \ell_{++}(\mathcal{G}(n,d)) \leq \ell_{+}(\mathcal{G}(n,d)) \leq \ell_{sch}(\mathcal{G}(n,d)),$$

and the bound $\ell_{++}(\mathcal{G}(n,d))$ is again expressed via a semidefinite program of size $O(n^3)$.

Summarizing, the parameters ℓ_{sch}, ℓ_{+}, ℓ_{++} 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 $\mathcal{X} \setminus \{\emptyset\}$ for ℓ_{sch}, by the set $\mathcal{X}$ for ℓ_+, and by the set $\mathcal{X}_+ = \mathcal{X} \cup \{\{I, V\} \mid I \in \mathcal{P}\}$ for ℓ_{++}. (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, $A(n,d) = \alpha(\mathcal{G}_{\rm ev}(n,d))$, the stability number of the graph $\mathcal{G}_{\rm ev}(n,d)$, defined as the subgraph of $\mathcal{G}(n,d)$ induced by the set

$$\mathcal{P}_{\rm ev} := \{I \subseteq V \mid |I| \text{ is even}\}.$$

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

$$y_{\mathcal{A}} = 0 \quad \text{if } \mathcal{A} \not\subseteq \mathcal{P}_{\rm ev} \tag{51}$$

for any $\mathcal{A} \in \mathcal{P}_{2k}(\mathcal{P})$ 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:

$$x^t_{i,j} = 0 \quad \text{if one of } i \text{ or } j \text{ is odd,} \tag{52}$$

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

$$z^t_{i,j} = 0 \quad \text{if one of } i, j, \text{ or } n \text{ is odd} \tag{53}$$

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

$$\ell^0(\mathcal{G}(n,d)) := \max\ 2^n x^0_{0,0} \ \text{ s.t. } x^t_{i,j}\ (i,j,t = 0,\ldots,n) \text{ satisfy } (35), (36), (39)(i)\text{–}(iii), (52) \tag{54}$$

and let ℓ^0_+, (resp., $\ell^0_{\rm sch}$, ℓ^0_{++}) be defined analogously by adding (52) (resp., (52), (52)–(53)) to (41) (resp., (42), (50)).

As $A(n,d) = \alpha(\mathcal{G}_{\rm ev}(n,d))$, $A(n,d)$ is bounded by the parameter $\ell(\mathcal{G}_{\rm ev}(n,d))$ (and analogously by $\ell_+(\mathcal{G}_{\rm ev}(n,d))$, $\ell_{++}(\mathcal{G}_{\rm ev}(n,d))$). The subgroup

$$G_{ev} := \{\pi s_A \mid A \in \mathcal{P}_{ev}\}$$

of the group G (introduced in (10)) acts vertex-transitively on $\mathcal{P}_{\rm ev}$. Hence, applying Lemma 3, $\ell(\mathcal{G}_{\rm ev}(n,d))$ 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 $\mathcal{P}_{\rm ev}$. Again, A belongs to the Bose–Mesner algebra and B belongs to the Terwilliger algebra; that is, for some scalars x_k, $x^t_{i,j}$, A (resp., B) is equal to the principal submatrix of $\sum_{k \text{ even}} x_k M_k$ (resp., of $\sum_{i,j,t \text{ even}} x^t_{i,j} M^t_{i,j}$) indexed by $\mathcal{P}_{\rm ev}$. Therefore, $\ell(\mathcal{G}_{ev}(n,d))$ can be computed via the program:

$$\ell(\mathcal{G}_{ev}(n,d)) = \max\ 2^{n-1}x^0_{0,0} \ \text{ s.t. } x^t_{i,j}\ (i,j,t = 0,\dots,n) \text{ satisfy } (35), (36), (39)(i)\text{–}(iii), (52) \tag{55}$$

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 5 $A(n,d) \le \ell(\mathcal{G}_{\rm ev}(n,d)) \le \ell^0(\mathcal{G}(n,d)) \le \ell(\mathcal{G}(n,d))$ *and analogously for the parameters* ℓ_+, $\ell_{\rm sch}$, ℓ_{++}.

Proof The right and left most inequalities are obvious. To compare the parameters $\ell(\mathcal{G}_{\rm ev}(n,d))$ 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 $\ell(\mathcal{G}_{\rm ev}(n,d))$. Thus y is indexed by $\mathcal{P}_3(\mathcal{P}_{ev})$, $y_{\{I,J\}} = 0$ if $|I \Delta J| = 1, \dots, d-1$ (for $I, J \in \mathcal{P}_{\rm ev}$) and, for any $I \in \mathcal{P}_{\rm ev}$, the matrix $Y_I(y)$ (indexed by $\mathcal{P}_2(\mathcal{P}_{ev}; I)$) 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 $\mathcal{A} \subseteq \mathcal{P}_{ev}$, 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 $\mathcal{P}_2(\mathcal{P}; I)$) is positive semidefinite. Thus, $\ell^0(\mathcal{G}(n,d)) \ge \sum_{I \in \mathcal{P}} z_I = \sum_{I \in \mathcal{P}_{ev}} y_I$, implying $\ell^0(\mathcal{G}(n,d)) \ge \ell(\mathcal{G}_{\rm ev}(n,d))$. The reasoning is analogous for the other parameters. □

The bound $\ell(\mathcal{G}_{\rm ev}(n,d))$ 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 $\ell_{\rm sch}(\mathcal{G}_{\rm ev}(n,d))$. For n odd, in view of (53), all variables $z^t_{i,j}$ can be set to 0 for the computation of $\ell_{++}(\mathcal{G}(n,d))$; from this follows that $\ell_+(\mathcal{G}_{\rm ev}(n,d)) = \ell_{++}(\mathcal{G}_{\rm ev}(n,d))$ 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 an 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, $\lfloor \ell_+(\mathcal{G}_{\rm ev}(25,6)) \rfloor$ and $\lfloor \ell_{++}(\mathcal{G}_{\rm ev}(20,8)) \rfloor$ 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 ℓ_+ and ℓ_{++} 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

Table 1 Comparing the bounds for $A(n,d)$

(n,d)	Delsarte bound	Schrijver bound $\ell_{\text{sch}}(\mathcal{G}_{\text{ev}}(n,d))$	$\ell_+(\mathcal{G}_{\text{ev}}(n,d))$	$\ell_{++}(\mathcal{G}_{ev}(n,d))$	$\ell^0_+(\mathcal{G}(n,d))$	$\ell^0_{++}(\mathcal{G}(n,d))$
(20,8)	290	274	274	273	274	273
(25,6)	48,148	47,998	47,997	47,997	47,998	47,998

`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.)

De Klerk and Pasechnik [1] have recently applied the bound of Schrijver [13] and our bound ℓ_+ 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 ℓ_+, replacing the constraint (36) by the constraint:

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

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 $n = 2 \mod 4$. 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

Table 2 Size of the semidefinite programs

Bound	# var.	# blocks	Block sizes
$\ell_+(\mathcal{G}_{ev}(25,6))$	131	27	13 14 12 12 11 11 10 10 9 9 8 8 7 7 6 6 5 5 4 4 3 3 2 2 1 1 -436
$\ell_+(\mathcal{G}_{ev}(20,8))$	43	23	11 12 9 9 9 9 7 7 7 7 5 5 5 5 3 3 3 3 1 1 1 1 -128
$\ell_{++}(\mathcal{G}_{ev}(20,8))$	68	12	34 27 27 21 21 15 15 9 9 3 3 -221

var. means 'number of variables',
blocks means 'number of blocks'

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

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

paper, where the bound ℓ_+ gave only a moderate improvement upon Schrijver's bound for the instances of the coding problem we have tested.

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