APPROXIMATING THE CHROMATIC NUMBER OF A GRAPH BY SEMIDEFINITE PROGRAMMING*

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Abstract. We investigate hierarchies of semidefinite approximations for the chromatic number $\chi(G)$ of a graph G. We introduce an operator Ψ mapping any graph parameter $\beta(G)$, nested between the stability number $\alpha(G)$ and $\chi\left(\overline{G}\right)$, to a new graph parameter $\Psi_\beta(G)$, nested between $\omega(G)$ and $\chi(G)$; $\Psi_\beta(G)$ is polynomial time computable if $\beta(G)$ is. As an application, there is no polynomial time computable graph parameter nested between the fractional chromatic number $\chi^*(\cdot)$ and $\chi(\cdot)$ unless P=NP and, based on Motzkin-Straus formulation for $\alpha(G)$, we give quadratic and copositive programming formulations for $\chi(G)$. Under some mild assumption, $n/\beta(G) \leq \Psi_\beta(G)$ but, while $n/\beta(G)$ remains below $\chi^*(G)$, $\Psi_\beta(G)$ can reach $\chi(G)$ (e.g., for $\beta(\cdot) = \alpha(\cdot)$). We define new lower bounds for $\chi(G)$ which we test on Hamming graphs and on some benchmark graphs. Our preliminary experimental results indicate that the new bounds can be much stronger than the classic bound $\vartheta\left(\overline{G}\right)$ (and its strengthenings obtained by adding nonnegativity and triangle inequalities).

Key words. chromatic number, semidefinite programming, block-diagonalization, Terwilliger algebra

AMS subject classifications. 05C15, 90C27, 90C22

1. Introduction. The chromatic number $\chi(G)$ of a graph $G = (V, E)$ is the minimum number of colors needed to color the nodes of G in such a way that adjacent nodes receive distinct colors. Computing $\chi(G)$ is an NP-hard problem [13] and it is also hard to approximate $\chi(G)$ within $n^{1/14-\epsilon}$ for any $\epsilon > 0$ [1] ($n := |V(G)|$). A well known lower bound for $\chi(G)$ is $\overline{\vartheta}(G) := \vartheta\left(\overline{G}\right)$, the theta number of the complementary graph, introduced by Lovász [20]. The theta number satisfies the 'sandwich inequality':

$$\omega(G) \leq \overline{\vartheta}(G) \leq \chi(G),$$

where $\omega(G)$ is the clique number of G, and can be computed to any arbitrary precision in polynomial time since it can be formulated via a semidefinite program. It can also be used for approximatively coloring the graph (see [5],[8],[12]). Intensive research has been done for strengthening the bound $\overline{\vartheta}(G)$ towards $\omega(G)$ or, equivalently, $\vartheta(G)$ towards the stability number $\alpha(G)$; see, e.g., [6, 16, 17, 18, 21, 22, 26, 29]. In particular, hierarchies of semidefinite (or linear) bounds were constructed that find $\alpha(G)$ in $\alpha(G)$ steps [16, 17, 21, 29]. As $\chi(G)$ can be formulated via a 0/1 linear program (see, e.g., [11]), the lift-and-project methods of [16],[21],[29] can in principle be applied to derive hierarchies of semidefinite approximations finding $\chi(G)$ in finitely many steps. To the best of our knowledge such hierarchies have not been investigated in detail so far.

In this paper we propose a systematic investigation of semidefinite approximations for $\chi(G)$. One of our main contributions is a simple construction permitting to derive from any graph parameter $\beta(G)$ nested between $\alpha(G)$ and $\overline{\chi}(G)$ a new graph parameter $\Psi_\beta(G)$ nested between $\omega(G)$ and $\chi(G)$. For this, let $G_l := K_l \square G$ denote the Cartesian product of G and K_l with node set

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$$V(G_l) := V(K_l) \times V(G) = \bigcup_{p=1}^{l} V_p, \quad \text{where } V_p := \{pi \mid i \in V\} \tag{1.1}$$

and having an edge (pi, qj) if $i = j$ or if ($p = q$ and $ij \in E(G)$). Obviously,

$$\chi(G) \leq l \Longleftrightarrow \alpha(G_l) = n. \tag{1.2}$$

This motivates defining $\Psi_\beta(G)$ as the smallest $l \in \mathbb{N}$ for which $\beta(G_l) = n$. Among other properties, $\Psi_\alpha(G) = \chi(G)$, $\Psi_{\overline{\chi}}(G) = \Psi_{\overline{\chi^*}}(G) = \omega(G)$, $\Psi_\vartheta(G) = \lceil \overline{\vartheta}(G) \rceil$, $\Psi_{\vartheta'}(G) = \left\lceil \overline{\vartheta^+}(G) \right\rceil$ (where ϑ', ϑ^+ are variations of ϑ obtained by adding certain nonnegativity conditions - see Section 2.1). Moreover, the operator Ψ is monotone nonincreasing, and if $\beta(G)$ is polynomial time computable (resp., given by a semidefinite program), then the same holds for $\Psi_\beta(G)$.

A somewhat surprising application is that there does *not* exist a polynomial time computable graph parameter nested between the fractional chromatic number and the chromatic number unless P=NP. As another application we can give quadratic and copositive programming formulations for $\chi(G)$ based on the Motzkin-Straus formulation for $\alpha(G)$. Our construction enables us to transform any hierarchy of upper bounds for $\alpha(G)$ into a hierarchy of lower bounds for $\chi(G)$. We study in particular hierarchies of lower bounds for $\chi(G)$ related to the Lasserre hierarchy $las^{(r)}(G)$ ($r \in \mathbb{N}$)[16], which finds $\alpha(G)$ at $r = \alpha(G)$ and refines several other known hierarchies for $\alpha(G)$.

We consider two hierarchies $\psi^{(r)}(G)$, $\Psi_{las^{(r)}}(G)$ which satisfy $\psi^{(1)}(G) = \overline{\vartheta}(G)$, $\psi^{(2)}(G) \geq \overline{\vartheta^{+\triangle}}(G)$ (Meurdesoif' strengthening), and

$$\frac{n}{las^{(r)}(G)} \leq \psi^{(r)}(G) \leq \Psi_{las^{(r)}}(G) \leq \chi(G).$$

The parameter $\psi^{(r)}(G)$ has the same computational cost as $las^{(r)}(G)$ but it cannot go beyond the fractional chromatic number (in fact, $\psi^{(r)}(G) = \chi^*(G)$ at $r \geq \alpha(G)$). The parameter $\Psi_{las^{(r)}}(G)$ has a higher computational cost than $las^{(r)}(G)$ (one has to evaluate $las^{(r)}(G_l)$ for $O(\log n)$ queries on $l \leq n$), but it finds $\chi(G)$ at step $r = n$. Dukanovic and Rendl [10] introduced recently another hierarchy for $\chi(G)$ using copositive programming; their bounds remain below the fractional chromatic number. At the time of writing this paper the details were not available, but it will be interesting later to investigate the connections between the various approaches.

Although polynomial time computable for any fixed r, the parameters $\psi^{(r)}(G)$, $\Psi_{las^{(r)}}(G)$ are yet too costly for large values of n already for $r = 2$. We propose some variations $\psi(G)$, $\Psi_\ell(G)$ of the order 2 bounds, at least as good as $\overline{\vartheta^+}(G)$. For vertex-transitive graphs, the computation of $\psi(G)$ involves a semidefinite program with one matrix of size $2n + 1$, while the computation of $\Psi_\ell(G)$ can be reduced to $O(\log n)$ semidefinite programs with matrices of sizes $2n+1, 2n, n, n$; this formulation is obtained by exploiting symmetries in the semidefinite program arising from the permutation group Sym(l) acting on K_l. We present numerical results for Hamming graphs $G = H(n, \mathcal{D})$ with $V(G) = \{0, 1\}^n$ and with an edge uv if the Hamming distance between u, v lies in $\mathcal{D}$. The Hamming graph G has a large automorphism group which enables us to reformulate the programs for $\psi(G)$, $\Psi_\ell(G)$ involving $O(n)$ matrices of size $O(n)$ (instead of 2^n!); as a crucial ingredient we use the block-diagonalization for the Terwilliger algebra given by Schrijver [28]. Finally we introduce a further variation $\psi_K(G)$ of our bounds (K clique in G) and see how it behaves on the Dimacs FullIns instances. In several instances, our lower bound is equal to the chromatic number, which indicates that the bounds are quite strong.

Contents of the paper. In Section 2 we describe the operator Ψ and its main properties, we discuss various ways for computing $\Psi_\beta(G)$ and give quadratic and copositive programming formulations for $\chi(G)$. In Section 3 we investigate two hierarchies of lower bounds for $\chi(G)$ related to the hierarchy of Lasserre for $\alpha(G)$ and converging respectively to $\chi^*(G)$ and $\chi(G)$. This leads to two bounds $\psi(G)$, $\Psi_\ell(G)$ formulated via semidefinite programs involving matrices of size $O(n)$. Section 4 is devoted to the computation of these two bounds for Hamming graphs; we show how to block-diagonalize the matrices in the semidefinite programs and report computational experiments. We describe in Section 5 another lower bound $\psi_K(G)$ which we test on the FullIns benchmark graphs.

Notation. Given a graph $G = (V, E)$, $\overline{G}$ denotes its complementary graph whose edges are the pairs $uv \notin E(G)$ ($u, v \in V(G)$, $u \neq v$). Throughout we set $V := V(G)$, $n = |V|$, and we assume that $G \neq K_n$, the complete graph on n nodes. For an integer $l \geq 1$, recall that $G_l = K_l \Box G$, the Cartesian product of G and K_l, whose node set is as in (1.1). Given a graph parameter $\beta(\cdot)$, $\overline{\beta}(\cdot)$ is the graph parameter defined by $\overline{\beta}(G) := \beta(\overline{G})$ for any graph G. Throughout, the letters $\mathbf{I}, \mathbf{J}, e$ denote, respectively, the identity matrix, the all-ones matrix, the all-ones vector (of the suitable size); $\mathbb{N}$ is the set of nonnegative integers. Given a finite set V, $\mathcal{P}(V)$ denote the collection of all subsets of V. Given an integer r, set $\mathcal{P}_r(V) := \{I \in \mathcal{P}(V) \mid |I| \leq r\}$. Given a vector $x \in \mathbb{R}^{\mathcal{P}(V)}$ we also set $x_i := x_{\{i\}}$, $x_{ij} := x_{\{i,j\}}$, $x_{ijk} := x_{\{i,j,k\}}$, etc. For $n \times n$ matrices A, B, $\mathrm{Tr}(A) = \sum_{i=1}^n A_{ii}$ and $\langle A, B \rangle = \mathrm{Tr}(A^T B) = \sum_{i,j=1}^n A_{ij} B_{ij}$.

Let V be a finite set and $\mathcal{G}$ be a subgroup of $\mathrm{Sym}(V)$, the group of permutations of V, also denoted as $\mathrm{Sym}(n)$ if $|V| = n$. $\mathcal{G}$ acts on $\mathcal{P}(V)$ by letting $\sigma(I) := \{\sigma(i) \mid i \in I\}$ for $I \subseteq V$, $\sigma \in \mathcal{G}$. Moreover, $\mathcal{G}$ acts on vectors and matrices indexed by V. Namely, for $M \in \mathbb{R}^{V \times V}$, $\sigma \in \mathcal{G}$, set $\sigma(M) := (M_{\sigma(i),\sigma(j)})_{i,j \in V}$; one says that M is invariant under action of $\mathcal{G}$ if $\sigma(M) = M$ for all $\sigma \in \mathcal{G}$; $\frac{1}{|\mathcal{G}|!} \sum_{\sigma \in \mathcal{G}} \sigma(M)$, the 'symmetrization' of M, is invariant under action of $\mathcal{G}$. Analogously for vectors. A semidefinite program is said to be invariant under action of $\mathcal{G}$ if, for any feasible matrix X and any $\sigma \in \mathcal{G}$, the matrix $\sigma(M)$ is again feasible with the same objective value; then the optimum value of the program remains unchanged if we restrict to invariant feasible solutions. Given a graph $G = (V, E)$ its automorphism group $\mathrm{Aut}(G)$ consists of all $\sigma \in \mathrm{Sym}(V)$ preserving the set of edges. Given $l, r \in \mathbb{N}$, we will often deal in the paper with semidefinite programs involving matrices indexed by $\mathcal{P}_r(V(G_l))$. Then the group $\mathrm{Sym}(l) \times \mathrm{Aut}(G)$ acts on such matrices and our programs will be invariant under this action.

2. New Parameters and Formulations.

2.1. The operator Ψ.

From (1.2) we see that the chromatic number of a graph G can be defined as the optimum solution of the following program

$$\chi(G) = \min_{l \in \mathbb{N}} l \ \text{ s.t. } \alpha(G_l) = n. \tag{2.1}$$

This motivates the following definition.

Definition 2.1. *Given a graph parameter $\beta(\cdot)$ satisfying*

$$\alpha(\cdot) \le \beta(\cdot) \le \overline{\chi}(\cdot), \tag{2.2}$$

define the graph parameter $\Psi_\beta(\cdot)$ by

$$\Psi_\beta(G) := \min_{l\in\mathbb{N}} l \quad s.t. \;\; \beta(G_l) = n.$$

Lemma 2.2. *The graph parameter $\Psi_\beta(G)$ is well defined if $\beta(\cdot)$ satisfies (2.2). The operator Ψ is monotone nonincreasing; that is, $\Psi_{\beta_2}(\cdot) \le \Psi_{\beta_1}(\cdot)$ if $\beta_1(\cdot)$, $\beta_2(.)$ satisfy (2.2) and $\beta_1(\cdot) \le \beta_2(\cdot)$. In particular,*

$$\Psi_\beta(G) \le \Psi_\alpha(G) = \chi(G).$$

Proof. From (2.2), for $1 \le l \le n$, $l \le \alpha(G_l) \le \beta(G_l) \le \overline{\chi}(G_l) \le n$. Hence, $\beta(G_n) = n$, which shows that $\Psi_\beta(G)$ is well defined. If $\beta_1(\cdot) \le \beta_2(\cdot)$ satisfy (2.2), then $\beta_1(G_l) = n$ implies $\beta_2(G_l) = n$, which gives $\Psi_{\beta_2}(G) \le \Psi_{\beta_1}(G)$. By (2.1), $\Psi_\alpha(G) = \chi(G)$, implying $\Psi_\beta(G) \le \Psi_\alpha(G) = \chi(G)$. □

Therefore, the operator Ψ takes a graph parameter $\beta(G)$ (nested between $\alpha(G)$ and $\overline{\chi}(G)$) and produces an integer lower bound $\Psi_\beta(G)$ for its chromatic number $\chi(G)$. As $\alpha(G)\chi^*(G) \ge n$, $\beta(G) \ge \alpha(G)$ implies $\chi(G) \ge \chi^*(G) \ge \frac{n}{\beta(G)}$. Consider the condition

$$\beta(G_l) \le l\beta(G) \quad \text{for all } l; \tag{2.3}$$

it holds for the graph parameters considered in the paper, e.g., for $\beta(\cdot) = \alpha(\cdot)$,$\chi(\cdot)$, $\chi^*(\cdot)$, $\vartheta(\cdot)$, $\vartheta'(\cdot)$, $las^{(r)}(\cdot)$. Under (2.3),

$$\Psi_\beta(G) \ge \frac{n}{\beta(G)}.$$

Thus $\Psi_\beta(G)$ improves the obvious lower bound $\frac{n}{\beta(G)}$ for $\chi(G)$. However, $\Psi_\beta(G)$ may be equal to $\chi(G)$ while $\frac{n}{\beta(G)}$ remains below the fractional chromatic number.

Next, we review some classic bounds for $\alpha(G)$ and $\chi(G)$ and investigate how the operator Ψ acts on them. First we recall their definitions.

• The fractional clique cover number (also known as the strong fractional stable set number of G, or the fractional chromatic number of $\overline{G}$) (see [27]):

$$\overline{\chi^*}(G) := \begin{array}{ll} \max & e^T x \\ \text{s.t.} & \sum_{i\in C} x_i \le 1 \ (C \text{ clique}) \\ & x \in \mathbb{R}^V_+ \end{array} = \begin{array}{ll} \min & e^T\lambda \\ \text{s.t.} & \sum_{C \text{ clique}} \lambda_C \chi^C = e \\ & \lambda \ge 0. \end{array} \tag{2.4}$$

• Lovász's theta number [20] (see also [19]):

$$\vartheta(G) := \begin{array}{ll} \max & \langle \mathbf{J}, X\rangle \\ \text{s.t.} & \mathrm{Tr}(X) = 1 \\ & X_{ij} = 0 \ \ (ij \in E(G)) \\ & X \succeq 0 \end{array} = \begin{array}{ll} \min & t \\ \text{s.t.} & U_{ii} = 1 \ (i \in V) \\ & U_{ij} = -\frac{1}{t-1} \ \ \left(ij \in E\left(\overline{G}\right)\right) \\ & U \succeq 0, \ t \ge 2. \end{array}$$

• The strengthening of the theta number of [26, 22]:

$$\begin{array}{llll} \vartheta'(G) := & \max & \langle \mathbf{J}, X\rangle & = & \min & t \\ & \text{s.t.} & \operatorname{Tr}(X) = 1 & & \text{s.t.} & U_{ii} = 1 \ (i \in V) \\ & & X_{ij} = 0 \ \ (ij \in E(G)) & & & U_{ij} \leq -\frac{1}{t-1} \ \ \left(ij \in E\left(\overline{G}\right)\right) \\ & & X \succeq 0, \ X \geq 0 & & & U \succeq 0, \ t \geq 2. \end{array}$$

• Szegedy's number [30]:

$$\begin{array}{llll} \vartheta^{+}(G) := & \max & \langle \mathbf{J}, X\rangle & = & \min & t \\ & \text{s.t.} & \operatorname{Tr}(X) = 1 & & \text{s.t.} & U_{ii} = 1 \ (i \in V) \\ & & X_{ij} \leq 0 \ \ (ij \in E(G)) & & & U_{ij} = -\frac{1}{t-1} \ \ \left(ij \in E\left(\overline{G}\right)\right) \\ & & X \succeq 0 & & & U_{ij} \geq -\frac{1}{t-1} \ \ (ij \in E(G)) \\ & & & & & U \succeq 0, \ t \geq 2. \end{array}$$

• Meurdesoif [23] defines the bound $\vartheta^{+\triangle}(G)$ obtained by adding the 'triangle inequalities' $U_{ij} + U_{jk} - U_{ik} \leq 1$ (for $ij, jk \in E$) to the above program defining $\vartheta^{+}(G)$. The above parameters satisfy

$$\alpha(G) \leq \vartheta'(G) \leq \vartheta(G) \leq \vartheta^{+}(G) \leq \vartheta^{+\triangle}(G) \leq \overline{\chi}(G).$$

The next theorem shows that the operator Ψ maps ϑ to $\left\lceil \overline{\vartheta} \right\rceil$, ϑ' to $\left\lceil \overline{\vartheta^{+}} \right\rceil$ and $\overline{\chi^{*}}$, $\overline{\chi}$ to the clique number ω.

THEOREM 2.3. *For any graph G the following holds:*
(a) $\Psi_{\overline{\chi^{*}}}(G) = \Psi_{\overline{\chi}}(G) = \omega(G)$,
(b) $\Psi_{\vartheta}(G) = \left\lceil \overline{\vartheta}(G) \right\rceil$,
(c) $\Psi_{\vartheta'}(G) = \left\lceil \overline{\vartheta^{+}}(G) \right\rceil$.

One can also verify that $\Psi_{\alpha^{*}}(G) = 2$ for any graph G with at least one edge, where $\alpha^{*}(G)$ is the fractional stable set number (see [27]) (although one cannot claim $\alpha^{*}(G) \leq \overline{\chi}(G)$). De Klerk et al. [5] consider a parameter closely related to Ψ_{ϑ} for which they can also show that it coincides with $\left\lceil \overline{\vartheta} \right\rceil$. Before proving the theorem, we mention a consequence of Theorem 2.3 (a) of independent interest, showing that there is no polynomial time computable bound lying between $\chi^{*}(G)$ and $\chi(G)$ unless P=NP.

COROLLARY 2.4. *If $\beta(\cdot)$ is a graph parameter satisfying $\overline{\chi^{*}}(\cdot) \leq \beta(\cdot) \leq \overline{\chi}(\cdot)$, then there is no algorithm permitting to compute $\beta(G)$ in time polynomial in $|V(G)|$ unless P=NP.*

Proof. Suppose one can compute $\beta(G)$ in time $f(n)$ where f is a polynomial in $n = |V(G)|$. Then one can compute $\Psi_{\beta}(G) = \omega(G)$ (by Lemma 2.2 and Theorem 2.3 (a)) in time $\sum_{l=1}^{n} f(ln)$, thus polynomial in n. Computing the clique number is however an NP-hard problem [13]. ☐

We need the following lemmas for the proof of Theorem 2.3.

LEMMA 2.5. *Let X be an $ln \times ln$ block matrix, having an $n \times n$ matrix A as its diagonal blocks, and an $n \times n$ matrix B as nondiagonal blocks, i.e.*

$$X = \underbrace{\begin{pmatrix} A & B & \dots & B \\ B & A & \dots & B \\ \vdots & \vdots & \ddots & \vdots \\ B & B & \dots & A \end{pmatrix}}_{\imath \text{ blocks}}. \tag{2.5}$$

Then, $X \succeq 0 \Longleftrightarrow A - B \succeq 0$ *and* $A + (l-1)B \succeq 0$.

Proof. We define an $ln \times ln$ matrix U_l having the same block structure as the matrix X. For $p, q = 1, \ldots, l$, let U_l^{pq} denotes the (p,q)-th block of U_l, which is defined by

$$U_l^{pq} := \begin{cases} \frac{1}{\sqrt{l}}\mathbf{I} & \text{if } p = 1 \text{ or } q = 1, \\ \left(\frac{1}{\sqrt{l}+l} - 1\right)\mathbf{I} & \text{if } p = q \geq 2, \\ \frac{1}{\sqrt{l}+l}\mathbf{I} & \text{otherwise.} \end{cases} \tag{2.6}$$

Here $\mathbf{I}$ stands for the identity matrix of order n. Notice that U_l is symmetric and orthogonal, i.e., $U_l(U_l)^T = \mathbf{I}$. Let $Y := (U_l)^T X U_l$. Then, $Y \succeq 0$ if and only if $X \succeq 0$ and a simple calculation gives

$$Y = \begin{bmatrix} A + (l-1)B & 0 & \ldots & 0 \\ 0 & A - B & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & A - B \end{bmatrix}, \tag{2.7}$$

which shows the lemma. □

Lemma 2.6. *For a positive semidefinite* $n \times n$ *matrix* X, $n\,Tr(X) \geq \langle \mathbf{J}, X\rangle$, *with equality if and only if* $X = c\mathbf{J}$ *for some nonnegative scalar* c.

Proof. As $X \succeq 0$, its entries satisfy $X_{ii} + X_{jj} \geq 2X_{ij}$ for all $i, j \in \{1, ..., n\}$. Thus, $n\sum_{i=1}^n X_{ii} \geq \sum_{i,j=1}^n X_{ij}$. Equality holds if and only if $X_{ii} + X_{jj} = 2X_{ij}$ for all i, j, which gives $X_{ii} = X_{jj} = X_{ij}$ for all i, j. □

Proof of Theorem 2.3. (a) As $\overline{\chi^*}(\cdot) \leq \overline{\chi}(\cdot)$, Lemma 2.2 implies $\Psi_{\overline{\chi}}(G) \leq \Psi_{\overline{\chi^*}}(G)$. For $l := \omega(G)$, we have $\overline{\chi^*}(G_l) = n$. Indeed, as G_l has the same clique number as G, letting $x := \frac{1}{l}e \in \mathbb{R}^{V(G_l)}$, we have $e^Tx = n$, $x(C) \leq 1$ for all cliques C of G_l and $x \geq 0$. This shows $\Psi_{\overline{\chi^*}}(G) \leq \omega(G)$. To show the inequality $\omega(G) \leq \Psi_{\overline{\chi}}(G)$, consider a clique C of size $\omega(G)$ in G. Given an integer l, let C_l denote the subset of $V(G_l)$ consisting of all the copies of the nodes in C. Thus $|C_l| = l|C|$ and C_l is covered by l cliques in G_l. As $V(G_l) \setminus C_l$ is covered by $n - \omega(G)$ cliques in G_l, it follows that $\overline{\chi}(G_l) \leq l + n - \omega(G)$. Therefore, $\overline{\chi}(G_l) = n$ implies $l \geq \omega(G)$ which shows $\Psi_{\overline{\chi}}(G) \geq \omega(G)$.

(b) Let (l, X) be a feasible solution for the program defining $\Psi_\vartheta(G)$; that is,

$$X \succeq 0,\ X_{uv} = 0\ (uv \in E(G_l)),\ \mathrm{Tr}(X) = 1,\ \langle \mathbf{J}, X\rangle = n. \tag{2.8}$$

Here the matrix X is indexed by $V(G_l) = \cup_{p=1}^l V_p$ (recall (1.1)). As the program (2.8) is invariant under action of the group Sym(l), one may assume that X is invariant under action of Sym(l). Then, X has the the block form (2.5). Using Lemma 2.5, (2.8) can be rewritten as

$$\begin{gathered} A - B \succeq 0,\ A + (l-1)B \succeq 0,\ A_{ij} = 0\ (ij \in E(G)),\ \mathrm{diag}(B) = 0, \\ \mathrm{Tr}(A) = \tfrac{1}{l},\ \langle \mathbf{J}, A + (l-1)B\rangle = \tfrac{n}{l}. \end{gathered} \tag{2.9}$$

Lemma 2.6 implies $A + (l-1)B = \frac{1}{nl}\mathbf{J}$. Setting $U := nl(A - B)$, we find

$$U = \frac{1}{l-1}(nl^2 A - \mathbf{J}). \tag{2.10}$$

One can verify that (l, U) is feasible for the program

$$\min\ l\ \text{ s.t. } \operatorname{diag}(U) = e,\ U_{ij} = -\tfrac{1}{l-1}\ (ij \in E(G)),\ U \succeq 0. \tag{2.11}$$

defining the parameter $\overline{\vartheta}(G)$ with $l \in \mathbb{N}$. Conversely, let (l, U) be feasible for (2.11) with l integer. Define the matrices A, B via the equations

$$A - B = \frac{1}{nl} U \ \text{ and } A + (l-1)B = \frac{1}{nl}\mathbf{J} \tag{2.12}$$

and let X be the corresponding block matrix as in (2.5). One can verify that (2.9) holds and thus (2.8) holds too. That is, (l, X) is feasible for (2.8). Hence,

$$\Psi_{\vartheta}(G) = \min_{l \in \mathbb{N}} l\ \text{ s.t. } \operatorname{diag}(U) = e,\ U \succeq 0,\ U_{ij} = -\frac{1}{l-1}\ (ij \in E(G)). \tag{2.13}$$

Therefore, $\Psi_{\vartheta}(G) \geq \lceil \overline{\vartheta}(G) \rceil$. Equality holds. To see it, set $l := \overline{\vartheta}(G)$ and take an optimal U for the program (2.11). The matrix $Y := \frac{l-1}{\lceil l \rceil - 1} U + \frac{\lceil l \rceil - l}{\lceil l \rceil - 1}\mathbf{I}$ is feasible for (2.13) with objective value l.

The proof of (c) is analogous to that of (b). Simply note that adding the condition $X \geq 0$ to (2.8) amounts to adding the condition $A, B \geq 0$ to (2.9) and thus, in view of (2.10), to adding the condition $U_{ij} \geq -\frac{1}{l-1}$ $(i, j \in V)$ to (2.13).

2.2. Semidefinite formulation for the new bounds. We consider here issues related to the computation of $\Psi_{\beta}(G)$. We assume throughout that $\beta(\cdot)$ satisfies (2.2). There is an obvious way to find $\Psi_{\beta}(G)$; namely, by computing $\beta(G_l)$ for each $l = 1, \ldots, n$. When $\beta(\cdot)$ is monotone nondecreasing (with respect to taking induced subgraphs), one can use binary search and it suffices to compute $\beta(G_l)$ for $O(\log n)$ instances of l.

LEMMA 2.7. *Assume*

$$\beta(G_l) \leq \beta(G_{l+1}) \text{ for all } l \in \mathbb{N}. \tag{2.14}$$

Then $\beta(G_l) = n \iff \Psi_{\beta}(G) \leq l$.

Proof. The 'only if' part follows from the definition of $\Psi_{\beta}(G)$. Assume $l_0 := \Psi_{\beta}(G) \leq l$. Then $\beta(G_{l_0}) = n \leq \beta(G_l)$ implying $\beta(G_l) = n$. □

Under assumption (2.14) one can use binary search for computing $\Psi_{\beta}(G)$. Namely, given $l_0 \in [1, n]$, compute $\beta(G_{l_0})$. There are two cases:
• Either $\beta(G_{l_0}) < n$. Then $\Psi_{\beta}(G) \geq l_0 + 1$ (by the above lemma) and we can now restrict the search to $l \in [l_0 + 1, n]$.
• Or $\beta(G_{l_0}) = n$. Then $\Psi_{\beta}(G) \leq l$ and we can restrict the search to $l \in [1, l_0]$.
Therefore, one can find $\Psi_{\beta}(G)$ by computing $\beta(G_l)$ for $O(\log n)$ queries of l.

Observe that one may restrict the range of search for l. Suppose we know a lower bound l_1 and an upper bound l_2 on $\chi(G)$; that is, $l_1 \leq \chi(G) \leq l_2$. Then we may assume $l \leq l_2$ in the definition of $\Psi_{\beta}(G)$ and if we add the condition $l \geq l_1$ then one still obtains a lower bound for $\chi(G)$. Therefore, we may restrict the binary search to $l \in [l_1, l_2]$. For instance, one can choose $l_1 = 3$ if G is not bipartite, or $l_1(G) = \omega(G)$, and $l_2 = \Delta(G) + 1$ (or even $\Delta(G)$ by Brook's theorem (see [27]) if G is not a clique or an odd circuit); $\Delta(G)$ being the maximum degree of G.

Next we show that $\Psi_{\beta}(G)$ can be formulated via a single semidefinite program when $\beta(\cdot)$ is given by a semidefinite program satisfying certain assumptions. Namely, our construction applies to the case when the semidefinite program defining $\beta(\cdot)$ involves at least one equality constraint of the form $\langle A, X\rangle = 1$ with $A \succeq 0$. Then one may assume without loss of generality that all other (in)equality constraints in the program are homogeneous, i.e., of the form $\langle B, X\rangle \geq 0$. (Write any equation $\langle B, X\rangle = 0$ as two opposite inequalities $\langle -B, X\rangle \geq 0$ and $\langle B, X\rangle \geq 0$.) So let us assume that the parameter $\beta(\cdot)$ can be expressed as

$$\beta(H) = \max\ \langle C(H), X(H)\rangle \ \text{ s.t. } \begin{array}{l} \langle A(H), X(H)\rangle = 1 \\ \mathcal{B}(H)(X(H)) \geq 0 \\ X(H) \succeq 0, \end{array} \tag{2.15}$$

where $C(H)$ and $A(H)$ are constant symmetric $n\times n$ matrices and $\mathcal{B}(H) : S_n \to \mathbb{R}^{d(H)}$ is a linear operator. Note that $d(\cdot)$ depends on H, e.g. $d(H) = 2|E(H)|$ in the formulation of $\vartheta(H)$. Moreover we assume that

$$A(H) \succeq 0 \text{ and } \langle A(H), X(H)\rangle = 0 \Longrightarrow \langle C(H), X(H)\rangle = 0. \tag{2.16}$$

Note that assumptions (2.14), (2.15), (2.16) hold, e.g., for $\vartheta(\cdot)$, or for the Lasserre hierarchy considered in Section 3.1. Recall that our operator Ψ maps $\beta(\cdot)$ in the following way:

$$\begin{array}{llll} \Psi_\beta(G) := & \min & l & = \ \min \ l \\ & \text{s.t.} & \beta(G_l) = n & \quad \text{s.t. } \ \langle C(G_l), X(G_l)\rangle = n \\ & & & \qquad\quad \langle A(G_l), X(G_l)\rangle = 1 \\ & & & \qquad\quad \mathcal{B}(G_l)(X(G_l)) \geq 0 \\ & & & \qquad\quad X(G_l) \succeq 0. \end{array} \tag{2.17}$$

Let us define

$$\Phi_\beta(G) := \min\ \sum_{l=1}^n l\langle A(G_l), X(G_l)\rangle \ \text{ s.t. } \begin{array}{l} \sum_{l=1}^n \langle C(G_l), X(G_l)\rangle = n \\ \sum_{l=1}^n \langle A(G_l), X(G_l)\rangle = 1 \\ \mathcal{B}(G_l)(X(G_l)) \geq 0 \ (l = 1, ..., n) \\ X(G_l) \succeq 0 \ (l = 1, ..., n). \end{array} \tag{2.18}$$

THEOREM 2.8. *Under assumptions (2.15) and (2.16),* $\Phi_\beta(G) = \Psi_\beta(G)$.

Proof. Take a feasible solution $(l, X(G_l))$ for the program (2.17) and for $k \neq l$ set $X(G_k) := 0$. In this way one obtains a feasible solution for (2.18) with the same objective value as (2.17), which shows $\Phi_\beta(G) \leq \Psi_\beta(G)$. Conversely, let $X(G_l)$ $(l = 1, ..., n)$ be a feasible solution for (2.18) and set $a_l := \langle A(G_l), X(G_l)\rangle$. Thus $a_l \geq 0$ since $A(G_l) \succeq 0$ (by assumption (2.16)) and $\sum_l a_l = 1$. Consider l for which $a_l > 0$. As $\left\langle A(G_l), \frac{X(G_l)}{a_l}\right\rangle = 1$, $\frac{X(G_l)}{a_l}$ is feasible for (2.15) (with $H = G_l$) which implies $\left\langle C(G_l), \frac{X(G_l)}{a_l}\right\rangle \leq \beta(G_l) \leq n$; moreover, equality $\left\langle C(G_l), \frac{X(G_l)}{a_l}\right\rangle = n$ implies $\beta(G_l) = n$ and thus $\Psi_\beta(G) \leq l$. Now we have

$$n = \sum_l \langle C(G_l), X(G_l)\rangle = \sum_{l|a_l>0} a_l \left\langle C(G_l), \frac{X(G_l)}{a_l}\right\rangle \leq \left(\sum_{l|a_l>0} a_l\right) n = n.$$

(Here we used assumption (2.16) for the second equality.) Therefore, equality holds throughout which implies $\Psi_\beta(G) \leq l$ whenever $a_l > 0$. Hence, $\sum_l la_l = \sum_{l|a_l>0} la_l \geq \Psi_\beta(G)(\sum_{l|a_l>0} a_l) = \Psi_\beta(G)$ which gives $\Phi_\beta(G) \geq \Psi_\beta(G)$. ∎

Hence, under the assumptions (2.15) and (2.16), the parameter $\Psi_\beta(G)$ can be formulated via the semidefinite program (2.18) which involves a block-diagonal matrix with diagonal blocks $X(G_1), \ldots, X(G_n)$, each $X(G_l)$ being the matrix variable involved in the program (2.15) for the graph $H = G_l$. For instance, if (2.15) involves a matrix variable of order $f(V(H))$, then (2.18) involves a block-diagonal matrix with block sizes $f(n), f(2n), \ldots, f(n^2)$. As explained above one can reduce the size of the program (2.18) by restricting the range of l in program (2.18) to $l \in [l_1, l_2]$ where $l_1 \leq \chi(G) \leq l_2$.

2.3. Copositive and quadratic formulations for $\chi(G)$. The technique used in Section 2.2 can also be applied to derive quadratic and copositive formulations for the chromatic number. Our starting point is the theorem of Motzkin and Straus [24] which, for a graph G with adjacency matrix A_G, asserts

$$\frac{1}{\alpha(G)} = \min \ x^T(\mathbf{I} + A_G)x \ \text{ s.t. } x \in \mathbb{R}_+^{V(G)}, \ e^T x = 1 \tag{2.19}$$

or, equivalently,

$$\alpha(G) = \min \ t \ \text{ s.t. } t(\mathbf{I} + A_G) - \mathbf{J} \text{ is copositive.} \tag{2.20}$$

A matrix X being *copositive* if $x^T X x \geq 0$ for all $x \geq 0$. Using (2.19) we can rewrite the program (2.1) as

$$\chi(G) = \ \min \ l \text{ s.t. } \ x_l^T(\mathbf{I} + A_{G_l})x_l = \tfrac{1}{n}, \ e_l^T x_l = 1, \ x_l \in \mathbb{R}_+^{V(G_l)}. \tag{2.21}$$

Here and below e_l denotes the all-ones vector in $\mathbb{R}^{V(G_l)}$. Using the idea from Section 2.2 let us define

$$\begin{array}{rcll} \Phi(G) & := & \min & \sum_{l=1}^n l(e_l^T x_l)^2 \\ & & \text{s.t.} & \sum_{l=1}^n (e_l^T x_l)^2 = 1 \\ & & & \sum_{l=1}^n x_l^T(\mathbf{I} + A_{G_l})x_l = \frac{1}{n}. \\ & & & x_l \in \mathbb{R}_+^{V(G_l)} \ (l = 1, \ldots, n). \end{array} \tag{2.22}$$

PROPOSITION 2.9. *$\Phi(G) = \chi(G)$.*

Proof. Taking a feasible solution (l, x_l) for the program (2.21) and setting $x_k = 0$ for $k \neq l$, we obtain a feasible solution for (2.22) with objective value l. Thus, $\Phi(G) \leq \chi(G)$. Conversely, let x_l $(l = 1, ..., n)$ be feasible for (2.22). Then

$$\frac{1}{n} = \sum_l x_l^T(\mathbf{I} + A_{G_l})x_l = \sum_{l | x_l \neq 0} \frac{x_l^T}{e_l^T x_l}(\mathbf{I} + A_{G_l})\frac{x_l}{e_l^T x_l}(e_l^T x_l)^2 \geq \frac{1}{n} \sum_{l | x_l \neq 0} (e_l^T x_l)^2 = \frac{1}{n}.$$

We have used $\frac{x_l^T}{e_l^T x_l}(\mathbf{I} + A_{G_l})\frac{x_l}{e_l^T x_l} \geq \frac{1}{\alpha(G_l)} \geq \frac{1}{n}$. Hence equality holds throughout, which implies $\alpha(G_l) = n$ if $x_l \neq 0$ and thus $\chi(G) \leq l$ if $x_l \neq 0$. Therefore,

$$\sum_l l(e_l^T x_l)^2 = \sum_{l | x_l \neq 0} l(e_l^T x_l)^2 \geq \chi(G) \sum_{l | x_l \neq 0} (e_l^T x_l)^2 = \chi(G).$$

This shows $\Phi(G) \geq \chi(G)$. ∎

Up to rescaling, we obtain the following quadratic programming formulation for $\chi(G)$:

$$\begin{array}{rcll}\chi(G) & = & \min & \frac{1}{n^2}\sum_{l=1}^n l(e_l^T x_l)^2 \\ & & \text{s.t.} & \sum_{l=1}^n (e_l^T x_l)^2 = n^2 \\ & & & \sum_{l=1}^n x_l^T(\mathbf{I}+A_{G_l})x_l = n \\ & & & x_l \in \mathbb{R}_+^{V(G_l)} \ (l=1,\ldots,n).\end{array} \tag{2.23}$$

It is not difficult to verify that the above program remains a formulation of $\chi(G)$ if we replace the condition $x_l \geq 0$ (for all l) by the condition x_l is 0/1 valued (for all l). Therefore this gives a 0/1 quadratic programming formulation for the chromatic number involving $O(n^3)$ variables.

Starting from (2.23), we can now derive a copositive programming formulation for $\chi(G)$. Namely, consider the program

$$\begin{array}{rcll}\Phi(G) & := & \min & \frac{1}{n^2}\sum_{l=1}^n l\langle \mathbf{J}_l, X_l\rangle \\ & & \text{s.t.} & \sum_{l=1}^n \langle \mathbf{J}_l, X_l\rangle = n^2 \\ & & & \sum_{l=1}^n \langle \mathbf{I}+A_{G_l}, X_l\rangle = n \\ & & & X_l \text{ completely positive (for all } l).\end{array} \tag{2.24}$$

Here and below $\mathbf{J}_l$ denotes the all-ones matrix of order $|V(G_l)|$. A matrix X is *completely positive* if it belongs to the dual of the cone of copositive matrices, i.e., if it can be written as $X = \sum_i x_i x_i^T$ for some $x_i \geq 0$.

PROPOSITION 2.10. $\Phi(G) = \chi(G)$.

Proof. The formulation (2.23) for $\chi(G)$ implies directly $\Phi(G) \leq \chi(G)$. Conversely, let X_l ($1 \leq l \leq n$) be a feasible solution for (2.24). Consider l for which $X_l \neq 0$. Say, $X_l = \sum_{i_l} x_{i_l} x_{i_l}^T$ where $x_{i_l} \geq 0$, $x_{i_l} \neq 0$ for all i_l. Thus $\lambda_{i_l} := \sqrt{\langle \mathbf{J}_l, x_{i_l}x_{i_l}^T\rangle} = e_l^T x_{i_l} > 0$. Set $y_{i_l} := \frac{x_{i_l}}{\lambda_{i_l}}$. By assumption, we have $\sum_l \langle n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l, X_l\rangle = 0$. By (2.20), each matrix $n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l$ is copositive, since $n \geq \alpha(G_l)$. This implies $\langle n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l, X_l\rangle = 0$ and thus $\langle n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l, x_{i_l}x_{i_l}^T\rangle = 0$ for all i_l. From this follows that $\langle \mathbf{I}+A_{G_l}, y_{i_l}y_{i_l}^T\rangle = \frac{1}{n}$ for all i_l. As $e_l^T y_{i_l} = 1$, y_{i_l} is feasible for the program (2.21), implying $\chi(G) \leq l$ whenever $X_l \neq 0$. Now, $(1/n^2)\sum_l l\langle \mathbf{J}_l, X_l\rangle \geq (1/n^2)\chi(G)\sum_l \langle \mathbf{J}_l, X_l\rangle = \chi(G)$, giving $\Phi(G) \geq \chi(G)$. ∎

Rewriting the condition $\sum_l \langle \mathbf{I}+A_{G_l}, X_l\rangle = n$ as $\sum_l \langle n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l, X_l\rangle = 0$, the dual conic program of (2.24) reads:

$$\max_{y,z}\ y \text{ s.t. } \frac{1}{n^2}(l-y)\mathbf{J}_l + z(n(\mathbf{I}+A_{G_l}) - \mathbf{J}_l) \text{ copositive for } 1 \leq l \leq n. \tag{2.25}$$

There is no duality gap since the program (2.25) is strictly feasible. Thus (2.25) is yet another formulation of $\chi(G)$. This opens the road to another type of hierarchy of relaxations for $\chi(G)$, obtained by approximating the copositive cone by tractable subcones as suggested by Parrilo [25] (this kind of approach for the stable set problem was studied in [6, 14]).

3. Semidefinite Approximations for $\chi^*(G)$, $\chi(G)$. We have seen in Section 2 how to construct semidefinite programming lower bounds for the chromatic number of a graph from semidefinite upper bounds on the stability number. Several hierarchies of semidefinite upper bounds for the stability number have been proposed in the literature; in particular in [6, 16, 21, 29]. These hierarchies were further studied and compared, e.g., in [14, 17]. It turns out that Lasserre's hierarchy, proposed in [16], gives the tightest bounds. For this reason we focus in this section on this hierarchy and show how it can be used and transformed to produce hierarchies of lower bounds for the (fractional) chromatic number.

3.1. Lasserre's hierarchy for the stability number. For a subset $I \subseteq V$ and an integer $r \geq 1$, define the vectors $\chi^S \in \{0,1\}^V$ with i-th entry 1 if and only if $i \in S$ (for $i \in V$), and $\chi^{S,r} \in \{0,1\}^{\mathcal{P}_r(V)}$ with I-th entry 1 if and only if $I \subseteq S$ (for $I \in \mathcal{P}_r(V)$). Given a vector $x = (x_I)_{I \in \mathcal{P}_{2r}(V)}$, consider the matrix:

$$M_r(x) := (x_{I \cup J})_{I,J \in \mathcal{P}_r(V)}$$

known as the *(combinatorial) moment matrix* of x of order r. By setting[1]:

$$las^{(r)}(G) := \max \sum_{i \in V} x_i \ \text{ s.t. } \ M_r(x) \succeq 0, \ x_\emptyset = 1, \ x_{ij} = 0 \ (ij \in E) \tag{3.1}$$

one obtains a hierarchy of semidefinite bounds for the stability number, known as Lasserre's hierarchy [16, 17]. Indeed, if S is a stable set, the vector $x := \chi^{S,2r}$ is feasible for (3.1) with objective value $|S|$, showing $\alpha(G) \leq las^{(r)}(G)$. We note that $las^{(1)}(G) = \vartheta(G)$. For fixed r, the parameter $las^{(r)}(G)$ can be computed in polynomial time (to an arbitrary precision) since the semidefinite program (3.1) involves matrices of size $O(n^r)$ with $O(n^{2r})$ variables.

It is shown in [17] that, for $r \geq \alpha(G)$, $M_r(x) \succeq 0$ if and only if x can be written as a convex combination of the vectors $\chi^{S,2r}$ (for $S \subseteq V$ stable set). This implies

$$\alpha(G) = las^{(r)}(G) \text{ for } r \geq \alpha(G). \tag{3.2}$$

3.2. A hierarchy of semidefinite bounds towards $\chi^*(G)$. For an integer $r \geq 1$, define the parameter

$$\psi^{(r)}(G) := \min \ l \ \text{ s.t. } \ M_r(x) \succeq 0, \ x_\emptyset = l, \ x_i = 1 (i \in V), \ x_{ij} = 0 \ (ij \in E) \tag{3.3}$$

with variable $x \in \mathbb{R}^{\mathcal{P}_{2r}(V)}$. For fixed r one can compute $\psi^{(r)}(G)$ to any arbitrary precision in polynomial time.

THEOREM 3.1. *The parameters $\psi^{(r)}(G)$ satisfy:*
(a) $\psi^{(r)}(G) \leq \psi^{(r+1)}(G)$,
(b) $\psi^{(1)}(G) = \overline{\vartheta}(G)$,
(c) $\psi^{(r)}(G) \leq \chi^*(G)$, with equality if $r \geq \alpha(G)$,
(d) $\psi^{(r)}(G) las^{(r)}(G) \geq n$, with equality if G is vertex-transitive.

Proof. (a) is easy. For (b), let $M_1(x) = \begin{pmatrix} l & e^T \\ e & M \end{pmatrix}$ be a matrix optimal for (3.3) with $r = 1$. Then $\psi^{(1)}(G) = l$ and $M_1(x) \succeq 0$ or, equivalently, $M - \frac{1}{l} ee^T \succeq 0$. After setting $U := \frac{l}{l-1}(M - \frac{1}{l} ee^T) = \frac{l}{l-1} M - \frac{1}{l-1} ee^T$, we can rewrite the program for $\psi^{(1)}(G)$ in the following way

$$\psi^{(1)}(G) = \min \ l \ \text{ s.t. } \ \begin{array}{l} U_{ii} = 1 \\ U_{ij} = -\frac{1}{l-1} \ (ij \in E) \\ U \succeq 0, \ l \geq 2. \end{array}$$

[1]One can easily verify that, under the condition $M_r(x) \succeq 0$, the edge condition: $x_{ij} = 0$ for $ij \in E$, implies that $x_I = 0$ for any $I \in \mathcal{P}_{2r}(V)$ containing an edge.

Thus $\psi^{(1)}(G) = \overline{\vartheta}(G)$.
(c) Let λ be an optimum solution for the program defining $\chi^*(G)$ (recall the left program in (2.4)). That is, $e^T\lambda = \chi^*(G)$, $\sum_{S \text{ stable}} \lambda_S \chi^S = e$ and $\lambda \geq 0$. For $r \in \mathbb{N}$, set $M := \sum_{S \text{ stable}} \lambda_S \chi^{S,r} \left(\chi^{S,r}\right)^T$. The matrix M is feasible for (3.3) with objective value $\chi^*(G)$ which shows $\psi^{(r)}(G) \leq \chi^*(G)$. Assume now $r \geq \alpha(G)$ and consider an optimum solution $M_r(x)$ for (3.3). Setting $y := \frac{1}{\psi^{(r)}(G)} x$, we have $M_r(y) \succeq 0$, $y_\emptyset = 1$, $y_{ij} = 0$ ($ij \in E$). By the result of [17] recalled before (3.2), $y = \sum_{S \text{ stable}} \lambda_S \chi^{S,2r}$ for some $\lambda_S \geq 0$ with $\sum_S \lambda_S = 1$. Rescaling and taking the projection onto the subspace $\mathbb{R}^V$, we find a decomposition $e = \psi^{(r)}(G) \sum_{S \text{ stable}} \lambda_S \chi^S$ with $\sum_S \lambda_S \psi^{(r)}(G) = \psi^{(r)}(G)$, which shows $\chi^*(G) \leq \psi^{(r)}(G)$.
(d) Take again an optimum solution $M_r(x)$ for (3.3). Since $M_r\left(\frac{1}{\psi^{(r)}(G)} x\right)$ is feasible for (3.1) with objective value $\frac{n}{\psi^{(r)}(G)}$, we get $las^{(r)}(G) \geq \frac{n}{\psi^{(r)}(G)}$. Assume that G is vertex-transitive. Then there exists an optimum solution x for (3.1) which is invariant under action of the automorphism group of G. In particular, $x_i = x_j$ for all $i, j \in V$ and thus $x_i = \frac{las^{(r)}(G)}{n}$ for all $i \in V$. Then the matrix $\frac{n}{las^{(r)}(G)} M_r(x)$ is feasible for (3.3), yielding $\psi^{(r)}(G) \leq \frac{n}{las^{(r)}(G)}$. ☐

3.3. The hierarchy of bounds $\Psi_{las^{(r)}}(G)$ towards $\chi(G)$. By applying the operator Ψ to the hierarchy $las^{(r)}(\cdot)$ (recalled in Section 3.1), we obtain the following hierarchy of lower bounds for $\chi(G)$:

$$\begin{array}{lll} \Psi_{las^{(r)}}(G) & = \min\ l \text{ s.t.} & las^{(r)}(G_l) = n \\ & = \min\ l \text{ s.t.} & y_\emptyset = 1,\ \sum_{u \in V(G_l)} y_u = n, \\ & & y_{uv} = 0\ (uv \in E(G_l)),\ M_r(y) \succeq 0 \end{array} \tag{3.4}$$

where the variable y is indexed by $\mathcal{P}_{2r}(V(G_l))$. As $las^{(n)}(G_l) = \alpha(G_l)$ for any $l \in \mathbb{N}$ (by (3.2)), (1.2) implies:

PROPOSITION 3.2. $\Psi_{las^{(n)}}(G) = \chi(G)$.

PROPOSITION 3.3. $\overline{\vartheta^{+\triangle}}(G) \leq \psi^{(2)}(G)$.

Proof. Assume (l, x) is feasible for the program defining $\psi^{(2)}(G)$. Consider the submatrix X of $M_2(x)$ indexed by $\{3, 12, 13, 23\}$ where $1, 2, 3$ are distinct elements of V and the vector $w := (1, 1, -1, -1)^T$. Then, $w^T X w \geq 0$ gives $x_{13} + x_{23} - x_{12} \leq 1$. Setting $U := \frac{l}{l-1}\left((x_{ij})_{i,j=1}^n - \frac{1}{l}\mathbf{J}\right)$, one can now verify that (l, U) is feasible for the program defining $\overline{\vartheta^{+\triangle}}(G)$, which shows the result. ☐

PROPOSITION 3.4. *For any integer $r \geq 1$, $\psi^{(r)}(G) \leq \Psi_{las^{(r)}}(G)$.*

Proof. Let (l, y) be feasible for the program defining the parameter $\Psi_{las^{(r)}}(G)$; that is, $y \in \mathbb{R}^{\mathcal{P}_{2r}(V(G_l))}$ satisfies $y_\emptyset = 1$, $y_{uv} = 0$ ($uv \in E(G_l)$), $\sum_{u \in V(G_l)} y_u = n$, and $M_r(y) \succeq 0$. We may assume w.l.o.g. that y is invariant under action of the symmetric group $\text{Sym}(l)$. The next claim determines y_u for $u \in V(G_l)$.

CLAIM 3.5. $y_u = \frac{1}{l}$ *for all $u \in V(G_l)$.*

Proof. Let X denote the principal submatrix of $M_r(y)$ indexed by $\{\emptyset\} \cup V(G_l)$. With respect to the partition of $\{\emptyset\} \cup V(G_l)$ into $\{\emptyset\} \cup (\cup_{p=1}^{l} V_p)$ (recall (1.1)), the matrix X has the block form

$$\begin{pmatrix} 1 & a^T & a^T & \dots & a^T \\ a & A & B & \dots & B \\ a & B & A & \dots & B \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a & B & B & \dots & A \end{pmatrix} \tag{3.5}$$

where $a = \text{diag}(A)$, $\text{diag}(B) = 0$, $A_{ij} = 0$ for $ij \in E(G)$, and $e^T a = \frac{n}{l}$. Moreover, by Lemma 2.5, $A+(l-1)B-laa^T \succeq 0$. This implies $\langle \mathbf{J}, A+(l-1)B\rangle \geq l(e^T a)^2 = \frac{n^2}{l}$. On the other hand, by Lemma 2.6, $\langle \mathbf{J}, A+(l-1)B\rangle \leq n\text{Tr}(A+(l-1)B) = n\text{Tr}(A) = \frac{n^2}{l}$. Hence equality holds, implying $A + (l-1)B = \frac{1}{l}\mathbf{J}$ and thus $a = \frac{1}{l}e$. This shows $y_u = \frac{1}{l}$ for all $u \in V(G_l)$. □

Define the vector $x \in \mathbb{R}^{\mathcal{P}_{2r}(V)}$ with I-th entry $x_I := ly_{\{pi|i\in I\}}$ for $I \in \mathcal{P}_{2r}(V)$ (where p is any fixed integer in $\{1,\dots,l\}$). Then, $M_r(x) \succeq 0$, since it coincides with the principal submatrix of $M_r(y)$ indexed by $\{\emptyset\} \cup \{\{pi \mid i \in I\} \mid I \in \mathcal{P}_r(V)\}$. Moreover, $x_\emptyset = l$ and $x_i = 1$ for $i \in V$. Thus, (l, x) is feasible for the program (3.3), which implies $\psi^{(r)}(G) \leq \Psi_{las^{(r)}}(G)$. □

3.4. Variations of the second order bounds $\psi^{(2)}(G)$, $\Psi_{las^{(2)}}(G)$. As observed in Propositions 3.3 and 3.4, we have

$$\overline{\vartheta^+}(G) \leq \overline{\vartheta^{+\triangle}}(G) \leq \psi^{(2)}(G) \leq \Psi_{las^{(2)}}(G).$$

We introduce some variations of the parameters $\psi^{(2)}(G)$ and $\Psi_{las^{(2)}}(G)$ which are at least as good as $\vartheta^+(G)$ but less costly to compute. The idea is to consider, instead of the full moment matrix of order 2, some principal submatrix of it. Following [18], define the following upper bound for $\alpha(G)$

$$\ell(G) := \max \sum_{i\in V} x_i \text{ s.t. } X_h(x) \succeq 0 \ (h \in V),\ x_\emptyset = 1,\ x_{ij} = 0 \ (ij \in E(G)) \tag{3.6}$$

where the variable x is indexed by $\mathcal{P}_3(V)$ and, for $h \in V$, $X_h(y)$ denotes the principal submatrix of $M_2(x)$ indexed by the subset $\mathcal{P}_1(V) \cup \{\{h,i\} \mid i \in V\}$ of $\mathcal{P}_2(V)$. Obviously,

$$las^{(2)}(G) \leq \ell(G) \leq las^{(1)}(G) = \vartheta(G).$$

Next, define the parameter

$$\psi(G) := \min\ l \text{ s.t. } \begin{array}{l} X_h(x) \succeq 0 \ (h \in V),\ x_{ij} = 0 \ (ij \in E(G)) \\ x_\emptyset = l,\ x_i = 1 \ (i \in V). \end{array} \tag{3.7}$$

Proposition 3.6. *We have*

$$\ell(G)\psi(G) \geq n, \text{ with equality if } G \text{ is vertex-transitive} \tag{3.8}$$

and

$$\overline{\vartheta^+}(G) \leq \psi(G) \leq \psi^{(2)}(G). \tag{3.9}$$

Proof. The proof for (3.8) is analogous to that of Theorem 3.1 (d) and the right inequality in (3.9) is obvious. For the left inequality, let (l, x) be feasible for (3.7) and let A denote the principal submatrix of $X_h(x)$ indexed by V. Then $A \geq 0$ and $A - \frac{1}{l}\mathbf{J} \succeq 0$, which implies that $U := \frac{l}{l-1}(A - \frac{1}{l}\mathbf{J})$ is feasible for the program defining $\overline{\vartheta^+}(G)$. ∎

By applying the operator Ψ to the parameter $\ell(\cdot)$, one obtains the lower bound $\Psi_\ell(G)$ for $\chi(G)$, defined as

$$\begin{aligned} \Psi_\ell(G) &= \min_{l\in\mathbb{N}}\ l \ \text{ s.t. } && \ell(G_l) = n \\ &= \min_{l\in\mathbb{N}}\ l \ \text{ s.t. } && \textstyle\sum_{u\in V(G_l)} y_u = n,\ y_{uv} = 0\ (uv \in E(G_l)), \\ & && y_\emptyset = 1,\ Y_u(y) \succeq 0\ (u \in V(G_l)) \end{aligned} \tag{3.10}$$

where the variable y is indexed by $\mathcal{P}_3(V(G_l))$.

Proposition 3.7. $\psi(G) \leq \Psi_\ell(G) \leq \Psi_{las^{(2)}}(G)$.

Proof. The right inequality is obvious and the proof for the left inequality is analogous to that of Proposition 3.4. ∎

For $l \in \mathbb{N}$, set

$$\Phi(G, l) := \min\ y_\emptyset \text{ s.t. } \quad \begin{aligned} \textstyle\sum_{u\in V(G_l)} y_u = n,\ y_{uv} = 0\ (uv \in E(G_l)), \\ Y_u(y) \succeq 0\ (u \in V(G_l)). \end{aligned} \tag{3.11}$$

Lemma 3.8. *For any integer $l \geq 1$, $\Phi(G, l) \geq 1$ and $\Phi(G, l+1) \leq \Phi(G, l)$.*

Proof. Let y be feasible for (3.11). We may assume w.l.o.g. that y is invariant under action of $\mathrm{Sym}(l)$. Let X denote the principal submatrix indexed by $\mathcal{P}_1(V_l)$ of $Y_u(y)$. Then, X has the block form (3.5) after replacing the entry 1 at the upper left corner by $y_\emptyset$. We have $e^T a = \frac{n}{l}$ and $\mathrm{diag}(B) = 0$. By Lemma 2.5, $A + (l-1)B - \frac{l}{y_\emptyset} aa^T \succeq 0$, which implies $\langle \mathbf{J}, A+(l-1)B\rangle \geq \frac{n^2}{l y_\emptyset}$. On the other hand, $\langle \mathbf{J}, A+(l-1)B\rangle \leq n\langle \mathbf{I}, A + (l-1)B\rangle = \frac{n^2}{l}$. From this follows that $y_\emptyset \geq 1$, which shows $\Phi(G, l) \geq 1$.

To show $\Phi(G, l+1) \leq \Phi(G, l)$, we observe that there exists $y' \in \mathbb{R}^{\mathcal{P}_3(V(G_{l+1}))}$ for which $(l+1, y')$ is feasible for the program (3.11) (with respect to the graph G_{l+1}) with $y'_\emptyset = y_\emptyset$. Namely, simply extend y to $\mathbb{R}^{\mathcal{P}_3(V(G_{l+1}))}$ by setting the new entries to 0. ∎

Lemma 3.9. *We have $\Psi_\ell(G) \leq l \iff \Phi(G, l) = 1$ and*

$$\Psi_\ell(G) = \min_{l\in\mathbb{N}}\ l \quad s.t. \quad \Phi(G, l) = 1. \tag{3.12}$$

Proof. If $\Phi(G, l) = 1$ then there exists a feasible solution (l, y) to the program (3.10), showing $\Psi_\ell(G) \leq l$. Conversely, assume $l_0 := \Psi_\ell(G) \leq l$. Then, there exists a feasible solution (l_0, y) to (3.10) with $y_\emptyset = 1$. Thus $\Phi(G, l_0) \leq 1$. Using Lemma 3.8, this implies $\Phi(G, l) = 1$. The reformulation (3.12) follows as a direct consequence. ∎

Therefore, as explained in Section 2.2, one can compute $\Psi_\ell(G)$ by evaluating $\Phi(G, l)$ for $O(\log n)$ queries of l. Given $l_0 \in [1, n]$, compute $\Phi(G, l_0)$ via (3.11). Either $\Phi(G, l_0) = 1$, then $\Psi_\ell(G) \leq l_0$ and restrict the search to $l \in [1, l_0]$; or $\Phi(G, l_0) > 1$, then $\Psi_\ell(G) \geq l_0 + 1$ and restrict the search to $l \in [l_0 + 1, n]$.

We now see how to give a more compact reformulation for the programs (3.10), (3.11) when G is a vertex-transitive graph. First, it suffices to require the condition

$Y_u(y) \succeq 0$ for *one* choice of $u \in V(G_l)$ (instead of for *all* $u \in V(G_l)$). Moreover, in the program (3.10) or (3.11), we may assume that the variable y is invariant under action of the group $\mathrm{Sym}(l) \times \mathrm{Aut}(G)$. Therefore we can write

$$\begin{array}{rl}\Psi_\ell(G) = \min\ l\ \text{ s.t.} & y_\emptyset = 1,\ y_u = \frac{1}{l}\ (u \in V(G_l)),\ y_{uv} = 0\ (uv \in E(G_l)), \\ & Y_{u_0}(y) \succeq 0,\ \sigma(y) = y\ \forall \sigma \in \mathrm{Sym}(l) \times \mathrm{Aut}(G).\end{array} \tag{3.13}$$

Here, $u_0 \in V(G_l)$ is fixed. From the invariance under action of the group $\mathrm{Sym}(l)$, it follows that the matrix $Y_{u_0}(y)$ is a block matrix with a very special structure.

LEMMA 3.10. *With respect to the partition $\{\emptyset\} \cup V_1 \cup \ldots \cup V_l \cup [\{u\} \times V_1] \cup \ldots \cup [\{u\} \times V_l]$, the matrix $Y_{u_0}(y)$ has the block form*

$$Y_{u_0}(y) = \begin{pmatrix} y_\emptyset & c^T & d^T \\ c & C & D \\ d & D & D \end{pmatrix}. \tag{3.14}$$

Here, $C, D \in \mathbb{R}^{nl \times nl}$, $c = \mathrm{diag}(C) \in \mathbb{R}^{nl}$, $d = \mathrm{diag}(D) \in \mathbb{R}^{nl}$,

$$C = \begin{pmatrix} A^1 & A^2 & \cdots & A^2 \\ A^2 & A^1 & \cdots & A^2 \\ \vdots & \vdots & \ddots & \vdots \\ A^2 & \cdots & \cdots & A^1 \end{pmatrix},\ D = \begin{pmatrix} B^1 & B^2 & B^2 & \cdots & B^2 \\ B^2 & B^3 & B^4 & \cdots & B^4 \\ B^2 & B^4 & B^3 & \cdots & B^4 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B^2 & B^4 & \cdots & \cdots & B^3 \end{pmatrix}, \tag{3.15}$$

where $A^1, \ldots, B^4 \in \mathbb{R}^{n \times n}$. Moreover, setting $a_1 := \mathrm{diag}(A^1)$, $b_1 := \mathrm{diag}(B^1)$, $b_3 := \mathrm{diag}(B^3)$, we have $a_1 = \frac{1}{l}e$, $c = [a_1^T \ldots a_1^T]^T$, $d = [b_1^T\, b_3^T\, b_3^T \ldots b_3^T]^T$.

To fix ideas, set $u_0 := 1h \in V_1$ (where $h \in V$). Then the entries of $A^1, \ldots, B^4$ are given by

$$\begin{array}{c} A^1_{ij} = y_{1i,1j},\ A^2_{ij} = y_{1i,2j},\ B^1_{ij} = y_{1i,1h,1j}, \\ B^2_{ij} = y_{1i,1h,2j},\ B^3_{ij} = y_{2i,1h,2j},\ B^4_{ij} = y_{2i,1h,3j} \end{array} \tag{3.16}$$

for $i, j \in V$. The edge constraints in the definition of the parameter $\Psi_\ell(G)$ can be reformulated as

$$\begin{array}{l} A^1_{ij} = 0 \text{ if } ij \in E(G), \\ B^1_{ij} = 0 \text{ if } \{i,j,h\} \text{ contains an edge of } G, \\ B^2_{ij} = 0 \text{ if } hi \in E(G) \text{ or } j \in \{i,h\}, \\ B^3_{ij} = 0 \text{ if } ij \in E(G) \text{ or if } h \in \{i,j\}, \\ B^4_{ij} = 0 \text{ if } h \in \{i,j\}, \\ \mathrm{diag}(A^2) = \mathrm{diag}(B^2) = \mathrm{diag}(B^4) = 0. \end{array} \tag{3.17}$$

The next lemmas indicate how one can block-diagonalize the matrix $Y_{u_0}(y)$.

LEMMA 3.11.

$$Y_{u_0}(y) \succeq 0 \Longleftrightarrow \begin{pmatrix} y_\emptyset - \frac{1}{l} & c^T - d^T \\ c - d & C - D \end{pmatrix} \succeq 0 \quad \textit{and} \quad D \succeq 0.$$

Proof. For this observe that the row of $Y_{u_0}(y)$ indexed by $\{u_0\}$ is equal to $(\frac{1}{l}, d^T, d^T)$. Some easy row/column manipulation gives the result (a similar idea was used in [18]). □

LEMMA 3.12. *We have*

$$D \succeq 0 \Longleftrightarrow \begin{pmatrix} B^1 & (l-1)B^2 \\ (l-1)(B^2)^T & (l-1)B^3 + (l-1)(l-2)B^4 \end{pmatrix},\ B^3 - B^4 \succeq 0.$$

Moreover,

$$\begin{pmatrix} y_\emptyset - \frac{1}{l} & c^T - d^T \\ c-d & C-D \end{pmatrix} \succeq 0 \Longleftrightarrow\ A^1 - B^3 - A^2 + B^4 \succeq 0 \quad \text{and}$$

$$\begin{pmatrix} y_\emptyset - \frac{1}{l} & \frac{1}{l}e^T - b_1^T & (l-1)(\frac{1}{l}e^T - b_3^T) \\ & A^1 - B^1 & (l-1)(A^2 - B^2) \\ & & (l-1)(A^1 - B^3) + (l-1)(l-2)(A^2 - B^4) \end{pmatrix} \succeq 0.$$

(We wrote only the upper triangular part in the above (symmetric) matrix.)

Proof. Consider the orthogonal matrices

$$M := \begin{pmatrix} \mathbf{I} & 0 \\ 0 & U_{l-1} \end{pmatrix},\ N := \begin{pmatrix} 1 & 0 \\ 0 & M \end{pmatrix}.$$

(Recall the definition of U_l from (2.6).) By the proof of Lemma 2.5,

$$MDM = \begin{pmatrix} B^1 & \sqrt{l-1}B^2 & 0 & \dots & 0 \\ \sqrt{l-1} & B^3 + (l-2)B^4 & 0 & \dots & 0 \\ 0 & 0 & B^3 - B^4 & & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & B^3 - B^4 \end{pmatrix}.$$

The first assertion of the lemma now follows after multiplying the second row/column block by $\sqrt{l-1}$. Next we have

$$N \begin{pmatrix} y_\emptyset - \frac{1}{l} & c^T - d^T \\ c-d & C-D \end{pmatrix} N = \begin{pmatrix} y_\emptyset - \frac{1}{l} & (c-d)^T M \\ M(c-d) & M(C-D)M \end{pmatrix}.$$

As the matrix $C - D$ has the same type of block shape as D, we deduce from the above that $M(C - D)M$ is block-diagonal. More precisely, the first diagonal block has the form

$$\begin{pmatrix} A^1 - B^1 & \sqrt{l-1}(A^2 - B^2) \\ \sqrt{l-1}(A^2 - B^2)^T & (A^1 - B^3) + (l-2)(A^2 - B^4) \end{pmatrix}$$

and the remaining $l-2$ diagonal blocks are all equal to $A^1 - B^3 - A^2 + B^4$. One can moreover verify that $(c-d)^T M = \left(\frac{1}{l}e^T - b_1^T, \sqrt{l-1}(\frac{1}{l}e^T - b_3^T), 0 \dots 0\right)$. From this follows the second assertion of the lemma. □

Summarizing, we have obtained the following more compact semidefinite program for the parameter $\Phi(G,l)$

$$\Phi(G,l) = \min\ y_\emptyset \ \text{ s.t. } \operatorname{diag}(A^1) = \frac{1}{l}e,\ b_1 = \operatorname{diag}(B^1),\ b_3 = \operatorname{diag}(B^3) \in \mathbb{R}^n,$$

$$A^1, B^1, B^2, B^3, B^4 \in \mathbb{R}^{n\times n} \text{ satisfy (3.17) and}$$

$$\begin{pmatrix} y_\emptyset - \frac{1}{l} & \frac{1}{l}e^T - b_1^T & (l-1)\left(\frac{1}{l}e^T - b_3^T\right) \\ & A^1 - B^1 & (l-1)(A^2 - B^2) \\ & & (l-1)(A^1 - B^3) + (l-1)(l-2)(A^2 - B^4) \end{pmatrix} \succeq 0,$$

$$\begin{pmatrix} B^1 & (l-1)B^2 \\ & (l-1)B^3 + (l-1)(l-2)B^4 \end{pmatrix} \succeq 0,$$

$$A^1 - A^2 - B^3 + B^4 \succeq 0,$$

$$B^3 - B^4 \succeq 0. \tag{3.18}$$

Thus $\Psi_\ell(G)$ can be obtained by computing $\Phi(G,l)$ for $O(\log n)$ queries of the parameter l, and the computation of each $\Phi(G,l)$ is via an SDP with four LMI's involving matrices of size $2n+1$, $2n$, n, n, respectively.

Let us finally note that one can easily strengthen the bound $\Psi_\ell(G)$, e.g., by requiring nonnegativity of the variables. Namely, let $\ell_{\geq 0}(G)$ (resp., $\psi_{\geq 0}(G)$) denote the variation of $\ell(G)$ (resp., $\psi(G)$) obtained by adding the condition $x \geq 0$ to (3.6) (resp., (3.7)); we have again $\psi_{\geq 0}(G)\ell_{\geq 0}(G) = |V(G)|$ when G is vertex-transitive. Define accordingly $\Psi_{\ell_{\geq 0}}(G)$, which amounts to requiring $y \geq 0$ in (3.10), (3.11), (3.13) and $A^1, \ldots, B^4 \geq 0$ in (3.18).

4. Bounds for Hamming graphs. We indicate here how to compute the parameters $\psi(G)$, $\Psi_\ell(G)$ when G is a Hamming graph. That is, given an integer $n \geq 1$ and $\mathcal{D} \subseteq V = \{1,\ldots,n\}$, G is the graph $H(n,\mathcal{D})$ with node set $V(G) := \mathcal{P}(V)$ and with an edge (I,J) if $|I\Delta J| \in \mathcal{D}$ (for $I,J \subseteq V$). Thus we now have $|V(G)| = 2^n$. In fact, $\psi(G) \geq \overline{\vartheta^{+\triangle}}(G)$ since one can verify that $\overline{\vartheta_+}(G) = \overline{\vartheta^{+\triangle}}(G)$ for Hamming graphs.

The program (3.18) involves matrices of size $O(2^n)$ and thus it cannot be solved directly for interesting values of n. However one can use the fact that the Hamming graph $G = H(n,\mathcal{D})$ has a large automorphism group for further reducing the size of the matrices $A^1, \ldots, B^3$ involved in the program (3.18). Namely, each permutation $\sigma \in \operatorname{Sym}(n)$ induces an automorphism of G, by letting $\sigma(I) := \{\sigma(i) \mid i \in I\}$ for $I \in \mathcal{P}(V)$; for $K \in \mathcal{P}(V)$, the *switching mapping* s_K defined by $s_K(I) := I\Delta K$ (for $I \in \mathcal{P}(V)$) is also an automorphism of G. Then $\operatorname{Aut}(G) = \{\sigma s_K \mid \sigma \in \operatorname{Sym}(n),\ K \in \mathcal{P}(V)\}$ and $|\operatorname{Aut}(G)| = n!2^n$.

It turns out that the blocks of the matrices in (3.18) belong to the Terwilliger algebra. Using the explicit block-diagonalization of the Terwilliger algebra, presented in Schrijver [28], we are able to block-diagonalize the matrices in (3.18) which enables the computation of $\Psi_\ell(G)$ for $G = H(n,\mathcal{D})$ for n up to 20. We recall the details needed for our treatment in the next subsection.

4.1. The Terwilliger algebra. For $i,j,t = 0,\ldots,n$, let $M_{i,j}^t$ denote the 0/1 matrix indexed by $\mathcal{P}(V)$ whose (I,J)-th entry is 1 if $|I| = i$, $|J| = j$, $|I\cap J| = t$, and equal to 0 otherwise. The set

$$\mathcal{A}_n := \left\{ \sum_{i,j,t=0}^{n} x_{i,j}^t M_{i,j}^t \mid x_{i,j}^t \in \mathbb{R} \right\}$$

is an algebra, known as the *Terwilliger algebra* of the Hamming graph. For $k = 0, \ldots, n$, let M_k be the matrix indexed by $\mathcal{P}(V)$ whose (I,J)-th entry is 1 if $|I \Delta J| = k$ and 0 otherwise. The set

$$\mathcal{B}_n := \left\{ \sum_{k=0}^{n} x_k M_k \mid x_k \in \mathbb{R} \right\}$$

is an algebra, known as the *Bose-Mesner algebra* of the Hamming graph. Obviously, $\mathcal{B}_n \subseteq \mathcal{A}_n$, since $M_k = \sum_{i,j,t|i+j-2t=k} M_{i,j}^t$. As is well known, $\mathcal{B}_n$ is a commutative algebra and thus all matrices in $\mathcal{B}_n$ can be simultaneously diagonalized (cf. Delsarte [4]). The Terwilliger algebra is not commutative, thus it cannot be diagonalized, however it can be block-diagonalized, as explained in [28]. We recall the main result below.

Given integers $i, j, k, t = 0, \ldots, n$, set

$$\beta_{i,j,k}^t := \sum_{u=0}^{n} (-1)^{t-u} \binom{u}{t} \binom{n-2k}{n-k-u} \binom{n-k-u}{i-u} \binom{n-k-u}{j-u}, \tag{4.1}$$

$$\alpha_{i,j,k}^t := \beta_{i,j,k}^t \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}}. \tag{4.2}$$

Theorem 4.1. *[28] For a matrix $M = \sum_{i,j,t} M_{i,j}^t x_{i,j}^t$ in the Terwilliger algebra,*

$$M \succeq 0 \Longleftrightarrow M_k := \left(\sum_t \alpha_{i,j,k}^t x_{i,j}^t \right)_{i,j=k}^{n-k} \succeq 0 \quad \text{for } k = 0, 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor. \tag{4.3}$$

To show this, Schrijver [28] constructs an orthogonal matrix U having the following property:

$$U^T M U = \begin{pmatrix} \widehat{M}_0 & 0 & \ldots & 0 \\ 0 & \widehat{M}_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \ldots & \widehat{M}_{\lfloor n/2 \rfloor} \end{pmatrix}, \quad \text{where } \widehat{M}_k = \begin{pmatrix} M_k & 0 & \ldots & 0 \\ 0 & M_k & \ldots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \ldots & M_k \end{pmatrix}$$

with block M_k being repeated $\binom{n}{k} - \binom{n}{k-1}$ times, for $k = 0, \ldots, \lfloor n/2 \rfloor$.

The result extends to a block matrix whose blocks all lie in the Terwilliger algebra and having a border of a special form. We state Lemma 4.2 for a 2×2 block matrix but the analogous result holds obviously for any number of blocks.

Lemma 4.2. *Let $A, B, C \in \mathcal{A}_n$; say, $A = \sum_{i,j,t} a_{i,j}^t M_{i,j}^t$, $B = \sum_{i,j,t} b_{i,j}^t M_{i,j}^t$, $C = \sum_{i,j,t} c_{i,j}^t M_{i,j}^t$ and define accordingly*

$$A_k = \left(\sum_t \alpha_{i,j,k}^t a_{i,j}^t \right)_{i,j=k}^{n-k}, \; B_k = \left(\sum_t \alpha_{i,j,k}^t b_{i,j}^t \right)_{i,j=k}^{n-k}, \; C_k = \left(\sum_t \alpha_{i,j,k}^t c_{i,j}^t \right)_{i,j=k}^{n-k}.$$

Then,

$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \succeq 0 \Longleftrightarrow \begin{pmatrix} A_k & B_k \\ B_k^T & C_k \end{pmatrix} \succeq 0 \ \forall k = 0, 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. Directly from the above using the orthogonal matrix $\begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}$. □

LEMMA 4.3. *(see Lemma 1 in [18]) Let $B = \sum_{i,j,t=0}^{t} x_{i,j}^t M_{i,j}^t \in \mathcal{A}_n$, $c = \sum_{i=0}^{n} c_i \chi^i$, where $\chi^i \in \{0,1\}^{\mathcal{P}(V)}$ with $\chi_I^i = 1$ if $|I| = i$ (for $I \in \mathcal{P}(V)$), and $d \in \mathbb{R}$. Then,*

$$\begin{pmatrix} d & c^T \\ c & B \end{pmatrix} \succeq 0 \Longleftrightarrow \begin{cases} B_k \succeq 0 \ \ \textit{for } k = 1, \ldots, \lfloor \frac{n}{2} \rfloor, \\ \tilde{B}_0 := \begin{pmatrix} d & \tilde{c}^T \\ \tilde{c} & B_0 \end{pmatrix} \succeq 0 \end{cases}$$

after setting $\tilde{c}^T := \left(c_i \sqrt{\binom{n}{i}} \right)_{i=0}^{n}$.

4.2. Compact formulation for $\psi(G)$ for Hamming graphs. As the graph $G = H(n, \mathcal{D})$ is vertex-transitive, we have $\psi(G) = \frac{2^n}{\ell(G)}$ by Proposition 3.6. It is shown in [18] how to compute the parameter $\ell(G)$ (when $\mathcal{D}$ is an interval $[1, d]$ but the reasoning is the same for any $\mathcal{D}$). The basic idea is that the matrix $X_h(x)$ appearing in (3.6) is a block matrix whose blocks lie in the Terwilliger algebra and thus it can be block-diagonalized. We recall the details, directly for the parameter $\psi(G)$, as they will be useful for our treatment of the parameter $\Psi_\ell(G)$ in the next section.

As G is vertex-transitive it suffices to require the condition $X_h(x) \succeq 0$ in (3.7) for *one* choice of $h \in V(G)$. Moreover, we may assume that the variable x is invariant under action of the automorphism group of G. To fix ideas, let us choose the node $h := \emptyset$ of G. With respect to the partition of its index set into $\{\emptyset\} \cup V(G) \cup \{\{\emptyset, I\} \mid I \in V(G)\}$, the matrix $X_\emptyset(x)$ has the block form

$$X_\emptyset(x) = \begin{pmatrix} l & e^T & b^T \\ e & A & B \\ b & B & B \end{pmatrix}. \tag{4.4}$$

where $\text{diag}(A) = e$ and $\text{diag}(B) = b$. Note that the row of $X_\emptyset(x)$ indexed by the singleton $\{\emptyset\}$ is equal to $(1, b^T, b^T)$ since $A_{\emptyset,J} = x_{\{\emptyset,J\}} = B_{\emptyset,J}$. Thus, using the same idea as for the proof of Lemma 3.11, we obtain

$$X_\emptyset(x) \succeq 0 \Longleftrightarrow \begin{pmatrix} l-1 & e^T - b^T \\ e - b & A - B \end{pmatrix} \succeq 0 \ \text{ and } \ B \succeq 0. \tag{4.5}$$

As x is invariant under action of $\text{Aut}(G)$, it follows that $A_{I,J} = x_{I,J} = x_{I',J'} = A_{I',J'}$ if $|I \Delta J| = |I' \Delta J'|$. In other words, the matrix A lies in the Bose-Mesner algebra; say,

$$A = \sum_{k=0}^{n} x_k M_k$$

for some reals x_k. Moreover, $B_{I,J} = x_{\emptyset,I,J} = x_{\emptyset,I',J'} = B_{I',J'}$ if $|I'| = |I|$, $|J'| = |J|$ and $|I' \cap J'| = |I \cap J|$. In other words, the matrix B lies in the Terwilliger algebra;

say,

$$B = \sum_{i,j,t=0}^{n} x^t_{i,j} M^t_{i,j}$$

for some reals $x^t_{i,j}$. The following holds for x_i, $x^t_{i,j}$.

LEMMA 4.4. *For $i, j, t = 0, \ldots, n$,*

$$\begin{array}{l} x_i = x^0_{0,i}, \\ x^t_{i,j} = x^t_{j,i} = x^{j-t}_{i+j-2t,j} = x^{i-t}_{i+j-2t,i} \end{array} \tag{4.6}$$

and the edge equations read

$$x^t_{i,j} = 0 \quad \text{if} \quad \{i, j, i+j-2t\} \cap \mathcal{D} \neq \emptyset. \tag{4.7}$$

Proof. If $|I| = i$, then $x_i = A_{\emptyset,I} = x_{\emptyset,I} = B_{\emptyset,I} = x^0_{0,i}$. Let $|I| = i$, $|J| = j$ and $|I \cap J| = t$. Then, $x^t_{i,j} = B_{I,J} = B_{J,I} = x^t_{j,i}$. Moreover, $x^t_{i,j} = B_{I,J} = x_{\emptyset,I,J} = x_{I,\emptyset,I\Delta J} = B_{I,I\Delta J} = x^{i-t}_{i+j-2t,i}$. This shows (4.6). The edge conditions read $B_{I,J} = x_{I,\emptyset,J} = 0$ if $\{|I|, |J|, |I\Delta J|\} \cap \mathcal{D} \neq \emptyset$, giving (4.7). ☐

We can now use the results from the previous subsection (Theorem 4.1 and Lemma 4.3) for block-diagonalizing the matrices occurring in (4.5). For $k = 0, \ldots, \lfloor n/2 \rfloor$, define the matrices

$$A_k := \left(\sum_t \alpha^t_{i,j,k} x^0_{0,i+j-2t} \right)^{n-k}_{i,j=k}, \quad B_k := \left(\sum_t \alpha^t_{i,j,k} x^t_{i,j} \right)^{n-k}_{i,j=k}$$

corresponding, resp., to A and B and set $\tilde{c} := \left(\sqrt{\binom{n}{i}} \left(1 - x^0_{0,i}\right) \right)^n_{i=0} \in \mathbb{R}^{n+1}$. The parameter $\psi(H(n, \mathcal{D}))$ can be reformulated in the following way:

$$\begin{array}{l} \psi(H(n,\mathcal{D})) = \min \ l \ \text{ s.t. } x^t_{i,j} \text{ satisfy (4.6), (4.7) and} \\ \qquad A_k - B_k \succeq 0 \ \text{ for } k = 1, \ldots, \lfloor n/2 \rfloor, \\ \qquad B_k \succeq 0 \ \text{ for } k = 0, 1, \ldots, \lfloor n/2 \rfloor, \\ \qquad \begin{pmatrix} l-1 & \tilde{c}^T \\ \tilde{c} & A_0 - B_0 \end{pmatrix} \succeq 0. \end{array} \tag{4.8}$$

4.3. Compact formulation for $\Psi_\ell(G)$ for Hamming graphs. We now give a more compact formulation for the parameter $\Psi_\ell(G)$ when $G = H(n, \mathcal{D})$. As explained in Lemma 3.9, one has to evaluate $\Phi(G, l)$ for various choices of l, with $\Phi(G, l)$ being given by (3.18). Recall the form of the entries of the matrices $A^1, \ldots, B^4$ from (3.16) (we fix again $h := \emptyset$). As for the parameter $\psi(H(n, \mathcal{D}))$ we now observe that $A^1, \ldots, B^4$ (and thus all blocks in the matrices in (3.18)) lie in the Terwilliger algebra.

LEMMA 4.5. *The matrices A^s ($s = 1, 2$) belong to the Bose-Mesner algebra and the matrices B^s ($s = 1, 2, 3, 4$) belong to the Terwilliger algebra. Say, $A^s = \sum_{i=0}^k x(s)_i M_i$ ($s = 1, 2$) and $B^s = \sum_{i,j,t=0}^k y(s)^t_{i,j} M^t_{i,j}$ ($s = 1, 2, 3, 4$). We have*

$$\begin{array}{c} x(1)_0 = \frac{1}{l}, \ x(s)_i = y(s)^0_{0,i} \ \textit{ for } s = 1, 2, \ i = 1, \ldots, n, \\[2ex] y(s)^t_{i,j} = y(s)^t_{j,i} = y(s)^{j-t}_{i+j-2t,j} = y(s)^{i-t}_{i+j-2t,i} \ (\textit{for } s = 1, 4), \\[2ex] y(2)^t_{i,j} = y(2)^{i-t}_{i,i+j-2t}, \ y(3)^t_{i,j} = y(3)^t_{j,i}, \\[2ex] y(3)^t_{i,j} = y(2)^{i-t}_{i+j-2t,i} \ \textit{ for } i, j, t = 0, \ldots, n. \end{array} \tag{4.9}$$

Moreover, the edge conditions can be reformulated as

$$\begin{array}{ll} y(1)^t_{i,j} = 0 & \text{if } \{i,j,i+j-2t\} \cap \mathcal{D} \neq \emptyset, \\ y(2)^i_{i,i} = y(4)^i_{i,i} = 0 & \text{for } i = 0,\ldots,n, \\ y(2)^t_{i,j} = 0 & \text{if } i \in \mathcal{D} \text{ or } j = 0, \\ y(3)^t_{i,j} = 0 & \text{if } i+j-2t \in \mathcal{D} \text{ or } i = 0 \text{ or } j = 0, \\ y(4)^t_{i,j} = 0 & \text{if } i = 0 \text{ or } j = 0. \end{array} \tag{4.10}$$

Proof. The details are similar to what was done in the previous section (e.g., Lemma 4.4) and are omitted. □

As the blocks of the matrices in the program (3.18) lie in the Terwilliger algebra, the matrices in (3.18) can be block-diagonalized, as explained in Section 4.1. For this, define the matrices

$$A^s_k := \left(\sum_t \alpha^t_{i,j,k} y(s)^0_{i+j-2t,0}\right)^{n-k}_{i,j=k}, \quad B^s_k := \left(\sum_t \alpha^t_{i,j,k} y(s)^t_{i,j}\right)^{n-k}_{i,j=k}$$

corresponding, respectively, to the matrices A^s $(s = 1,2)$ and B^s $(s = 1,2,3,4)$ and set

$$\tilde{a} := \left(\sqrt{\binom{n}{i}}\left(\frac{1}{l} - y(1)^i_{i,i}\right)\right)^n_{i=0}, \quad \tilde{b} := \left(\sqrt{\binom{n}{i}}\left(\frac{1}{l} - y(3)^i_{i,i}\right)\right)^n_{i=0} \in \mathbb{R}^{n+1}.$$

Using Lemmas 4.2 and 4.3, we obtain the following reformulation for the parameter $\Phi(G,l)$ from (3.18)

$$\Phi(G,l) = \min\ y_\emptyset \ \text{ s.t. } y(1)^t_{i,j}, y(2)^t_{i,j}, y(3)^t_{i,j}, y(4)^t_{i,j} \text{ satisfy (4.9), (4.10) and}$$

$$\begin{pmatrix} y_\emptyset - \frac{1}{l} & \tilde{a}^T & (l-1)\tilde{b}^T \\ & A^1_0 - B^1_0 & (l-1)(A^2_0 - B^2_0) \\ & & (l-1)(A^1_0 - B^3_0) + (l-1)(l-2)(A^2_0 - B^4_0) \end{pmatrix} \succeq 0,$$

$$\begin{pmatrix} A^1_k - B^1_k & (l-1)(A^2_k - B^2_k) \\ & (l-1)(A^1_k - B^3_k) + (l-1)(l-2)(A^2_k - B^4_k) \end{pmatrix} \succeq 0 \text{ for } k = 1,\ldots,\lfloor n/2 \rfloor,$$

$$\begin{pmatrix} B^1_k & (l-1)B^2_k \\ & (l-1)B^3_k + (l-1)(l-2)B^4_k \end{pmatrix} \succeq 0 \ \text{ for } k = 0,\ldots,\lfloor n/2 \rfloor,$$

$$A^1_k - A^2_k - B^3_k + B^4_k \succeq 0 \ \text{ for } k = 0,\ldots,\lfloor n/2 \rfloor,$$

$$B^3_k - B^4_k \succeq 0 \ \text{ for } k = 0,\ldots,\lfloor n/2 \rfloor. \tag{4.11}$$

4.4. Numerical results for Hamming graphs. We have tested the various bounds on some instances of Hamming graphs. In what follows we use the following convention: For an integer $1 \leq d \leq n$, $H(n,d)$ (resp., $H^-(n,d)$, $H^+(n,d)$) denotes the graph $H(n,\mathcal{D})$ with $\mathcal{D} = \{d\}$ (resp., $\mathcal{D} = \{1,\ldots,d\}$, $\{d,\ldots,n\}$). The recent paper [9] gives numerical results for the parameters $\overline{\vartheta}(G)$, $\overline{\vartheta^+}(G)$ for such instances. No instances with n larger than 12 are reported in [9]; note that the authors use symmetry reduction to reduce the number of variables but work with the full matrices of order 2^n.

The results in Table 1 below indicate that the parameters $\psi(G)$ and $\psi_{\geq 0}(G)$ give on some instances a major improvment on $\overline{\vartheta^+}(G)$. On the other hand, in most cases, the parameter $\Psi_\ell(G)$ gives no improvement since $\Psi_\ell(G) = \lceil \psi(G) \rceil$. It could be that this feature is specific to Hamming graphs.

In Table 1, the symbol '@' indicates the strict inequality $\Psi_\ell(G) > \lceil \psi(G) \rceil$. The symbol '*' indicates that LB $= \chi(G)$ for the obtained lower bound LB. (Indeed in these instances, LB $= 2^{n-1}$, while $\mathcal{P}(V)$ can be covered by the 2^{n-1} distinct pairs $\{I, V \setminus I\}$ $(I \subseteq V)$ which are stable sets as $n \notin \mathcal{D}$.)

graph	$\overline{\vartheta}(G)$	$\overline{\vartheta^+}(G)$	$\psi(G)$	$\Psi_\ell(G)$	$\psi_{\geq 0}(G)$	$\Psi_{\ell_{\geq 0}}(G)$
$H^-(7,4)$	36	42.6667	64	64	64	64*
$H^-(8,5)$	72	85.3333	128	128	128	128*
$H(10,6)$	6	8.7273	10.4366	11	10.8936	11
$H^-(10,6)$	207.36	320	512	512	512	512*
$H(10,8)$	2.6667	3.2	3.9232	$5^@$	3.9232	$5^@$
$H^+(10,8)$	3.2	3.2	3.9232	$5^@$	3.9232	$5^@$
$H(11,4)$	16	21.5652	25.7351	26	25.7351	26
$H(11,6)$	12	12	12	12	15.2836	16
$H^-(11,7)$	414.72	640	1024	1024	1024	1024*
$H^-(11,8)$	711.1111	819.2	1024	1024	1024	1024*
$H(11,8)$	3.2	4.9383	5.7805	6	5.7805	6
$H(13,8)$	5.3333	9.4118	12.1429	13	13.6533	14
$H(15,6)$	27.7647	30.7368	46.4371	47	50.3036	51
$H(16,8)$	16	16	16	16	28.4444	29
$H(17,6)$	35	48.2222	86.3086	87	88.3204	89
$H(17,8)$	18	18	32	32	46.5122	47
$H(17,10)$	6.6666	12.6315	15.8750	16	25.8405	26
$H(18,10)$	10	16	18.3076	19	38.8844	-
$H(20,6)$	59.3735	59.3735	140.9586	141	140.9586	-
$H(20,8)$	41.7143	60.9524	107.1489	-	136.4115	-

Table 1

5. Numerical Results for Benchmark Graphs. We have also conducted some preliminary experiments for some Dimacs benchmark graphs, namely on the FullIns instances. The chromatic number of these instances is known (see [2, 3, 7]). On several instances, we obtain a lower bound equal to the chromatic number, which demonstrates that our bounds are quite strong.

We have in fact used yet another variant of the bound $\psi^{(2)}(G)$. Namely, given a clique K in G, let $X_K(x)$ denote the principal submatrix of $M_2(x)$ indexed by the set $\mathcal{P}_1(V) \cup (\cup_{h \in K} \{\{h, i\} \mid i \in V\})$. Now define the parameter

$$\psi_K(G) := \min\ l \ \text{ s.t. } \ x_\emptyset = l,\ x_i = 1\ (i \in V),\ x_{ij} = 0\ (ij \in E(G)),\ X_K(x) \succeq 0. \quad (5.1)$$

Then $\overline{\vartheta}(G) \leq \psi_K(G) \leq \chi^*(G)$. Set $k := |K|$. With respect to the partition of its index set, the matrix $X_K(x)$ has the block form

$$X_K(x) = \begin{pmatrix} l & a_0^T & a_1^T & a_2^T & \dots & a_k^T \\ a_0 & A^0 & A^1 & A^2 & \dots & A^k \\ a_1 & A^1 & A^1 & 0 & \dots & 0 \\ a_2 & A^2 & 0 & A^2 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ a_k & A^k & 0 & \dots & 0 & A^k \end{pmatrix}$$

with $a_i = \mathrm{diag}(A^i)$ $(0 \le i \le k)$, $a_0 = e$, $A^0_{ij} = x_{ij}$, $A^h_{ij} = x_{\{h,i,j\}}$ for $h \in K$, $i, j \in V$. Using similar ideas as in Section 3.4, one can verify that

$$X_K(x) \succeq 0 \Longleftrightarrow \begin{pmatrix} l - k & e^T - (\sum_{h=1}^k a_h)^T \\ e - \sum_{h=1}^k a_h & A^0 - \sum_{h=1}^k A^h \end{pmatrix} \succeq 0, \; A^1, \dots, A^k \succeq 0.$$

Hence $\psi_K(G)$ can be computed via a semidefinite program involving matrices of sizes $n+1, n, \dots, n$ (k times).

In Table 2 below the column '$\chi(G)$' contains the chromatic number. The column 'lower bound' contains the value of $\psi_K(G')$, where G' is an induced subgraph of G. The symbol '*' indicates that our lower bound is equal to $\chi(G)$.

graph	nodes	edges	$\chi(G)$	lower bound
2-FullIns-4	212	1621	6	6 *
2-FullIns-5	852	12201	7	6
3-FullIns-4	405	3524	7	7 *
3-FullIns-5	2030	33751	8	7
4-FullIns-4	690	6650	8	8 *
4-FullIns-5	4146	77305	9	8
5-FullIns-4	1085	11395	9	9 *

Table 2

Let us explain how we have obtained our new lower bound for the instances in Table 2, the number of nodes of the graphs G appearing in the table being too large for allowing a direct computation of $\psi_K(G)$. The details for some of the above instances are given in Table 3 below. We have applied the following preprocessing procedure, which is commonly used in the literature for identifying an induced subgraph of G with the same chromatic number; see, e.g., [8].

Step 1. Determine a lower bound p on the chromatic number $\chi(G)$. (E.g., find a clique of size p.)

Step 2. Apply iteratively the following two rules:
• Delete a node u with $\deg(u) < p$;
• Delete a node u if there exists a node v for which $uv \notin E$ and $N(u) \subseteq N(v)$. (Here $N(u) := \{v \in V \mid uv \in E\}$, $\deg(u) = |N(u)|$.) Each such operation does not change the chromatic number of the graph. Let G_1 be the graph returned.

Step 3. Compute $\overline{\vartheta}(G_1)$. Thus $\overline{\vartheta}(G_1) \le \chi(G_1) = \chi(G)$. Apply again Step 2 with $p := \lceil \overline{\vartheta}(G_1) \rceil$. Let G_2 be the graph returned.

Step 4. Find a clique K in G_2 and compute $\psi_K(G_2)$. Thus $\psi_K(G_2) \le \chi(G_2) = \chi(G)$.

graph G	$\lvert V(G)\rvert$ $\lvert E(G)\rvert$	p	$\lvert V(G_1)$ $(G_1)\rvert$	$\vartheta(\overline{G_1})$ $\to p$	$\lvert V(G_2)\rvert$ $\lvert E(G_2)\rvert$	$\lvert K\rvert$	$\psi_K(G_2)$
2-FullIns-4	212 1621	4	41 161	4.056 5	31 141	4	5.456
3-FullIns-5	2030 33751	5	103 726	5.047 6	91 672	5	6.45
4-FullIns-4	690 6650	6	37 216	6.02 7	27 166	6	7.122
4-FullIns-5	4146 77305	6	113 926	6.03 7	99 852	6	7.452
5-FullIns-4	1085 11395	7	43 294	7.014 8	31 225	7	8.0873

Table 3: Details on the preprocessing phase

The computational results reported in this paper were carried out using the open source codes for semidefinite programming CSDP 5.0 and DSDP 5.8 available, respectively, at `http://infohost.nmt.edu/~borchers/csdp.html` and `http://www-unix.mcs.anl.gov/~benson/dsdp/`. For the computation of ϑ in Table 3 we have used the code of Dukanovic and Rendl, available at `http://www.math.uni-klu.ac.at/or/Software/`. Our results seem to indicate that the new bounds are quite powerful. Of course these are only preliminary experiments and we intend to further investigate how the ideas presented in the paper can be used for tackling larger coloring problems.

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REFERENCES

[1] Bellare, M., Sudan, M. 1994. $\chi(G)$ is not approximable within $|G|^{1/14-\epsilon}$. Proceedings of the 26th Annual ACM Symposium on Theory of Computing, 184–193.

[2] Caramia, M., Dell'Olmo, P. 2004. Bounding vertex coloring by truncated multistage branch and bound. *Networks*, 44:231–242.

[3] Chiarandini, M. 2005. *Stochastic Local Search Methods for Highly Constrained Combinatorial Optimisation Problems.* PhD thesis, Darmstadt University of Technology.

[4] Delsarte, P. 1973. *An Algebraic Approach to the Association Schemes of Coding Theory.* [Philips Research Reports Supplements (1973) No. 10] Philips Research Laboratories, Eindhoven.

[5] De Klerk, E., Pasechnik, D.V., Warners, J.P. 2004. On approximate graph colouring and MAX-k-CUT algorithms based on teh ϑ-function. *Journal of Combinatorial Optimization*, 8:267–294.

[6] De Klerk, E., Pasechnik, D.V. 2002. Approximating the stability number of a graph via copositive programming. *SIAM Journal on Optimization*, 12:875–892.

[7] Desrosiers, C., Galinier, P., Hertz, A. 2004. Efficient algorithms for finding critical subgraphs. Preprint.

[8] Dukanovic, I., Rendl, F. 2005. A semidefinite programming based heuristic for graph coloring. Preprint.

[9] Dukanovic, I., Rendl, F. 2005. Semidefinite programming relaxations for graph coloring and maximal clique problems. Preprint.

[10] Dukanovic, I., Rendl, F. 2005. Copositive programming motivated bounds on the clique and the chromatic number. Working paper.

[11] Diaz, I.M., Zabala, P. 2002. A branch-and-cut algorithm for graph coloring. Preprint.

[12] Karger, D., Motwani, R., Sudan, M. 1998. Approximate graph coloring by semidefinite programming. *Journal of the ACM*, 45:246–265.

[13] Garey, M.R., Johnson, D.S. 1979. *Computers and Intractability: A Guide to the Theory of NP-Completeness.* Freeman, San Francisco.

[14] Gvozdenović, N., Laurent, M. 2005. Semidefinite bounds for the stability number of a graph via sums of squares of polynomials. In M. Jünger and V. Kaibel (eds.), *Lecture Notes in Computer Science*, 3509:136-151.

[15] Lasserre, J.B. 2001. Global optimization with polynomials and the problem of moments. *SIAM Journal on Optimization*, 11:796–817.

[16] Lasserre, J.B. 2001. An explicit exact SDP relaxation for nonlinear $0-1$ programs. In K. Aardal and A.M.H. Gerards (eds.), *Lecture Notes in Computer Science*, 2081:293–303.

[17] Laurent, M. 2003. A comparison of the Sherali-Adams, Lovász-Schrijver and Lasserre relaxations for $0-1$ programming. *Mathematics of Operations Research*, 28:470–496.

[18] Laurent, M. 2005. Strengthened semidefinite programming bounds for codes. To appear in *Mathematical Programming.*

[19] Laurent, M., Rendl, F. 2005. Semidefinite programming and integer programming. In K. Aardal, G. Nemhauser, R. Weismantel (eds.), *Handbook on Discrete Optimization*, pp 393–514, Elsevier B.V.

[20] Lovász, L. 1979. On the Shannon capacity of a graph. *IEEE Transactions on Information Theory*, 25:1–7.

[21] Lovász, L., Schrijver, A. 1991. Cones of matrices and set-functions and $0-1$ optimization. *SIAM Journal on Optimization*, 1:166–190.

[22] R.J. McEliece, R.J., Rodemich, E.R., Rumsey, H.C., 1978. The Lovász' bound and some generalizations. *Journal of Combinatorics, Information & System Sciences*, 3:134–152.

[23] Meurdesoif, P. 2005. Strengthening the Lovász $\theta\left(\overline{G}\right)$ bound for graph coloring. *Mathematical Programming*, 102:577–588.

[24] Motzkin, T.S., Straus, E.G., 1965. Maxima for graphs and a new proof of a theorem of Túran. *Canadian Journal of Mathematics*, 17:533-540.

[25] Parrilo, P. 2000. *Structured Semidefinite Programs and Semialgebraic Geometry Methods in Robustness and Optimization.* PhD thesis, California Institute of Technology.

[26] Schrijver, A. 1979. A comparison of the Delsarte and Lovász bounds. *IEEE Transactions on Information Theory*, 25:425–429.

[27] Schrijver, A. 2003. *Combinatorial Optimization - Polyhedra and Efficiency*, Springer-Verlag, Berlin.

[28] Schrijver, A. 2005. New code upper bounds from the Terwilliger algebra and semidefinite programming. *IEEE Transactions on Information Theory*, 51:2859–2866.

[29] Sherali, H.D., Adams, W.P. 1990. A hierarchy of relaxations and convex hull characterizations for mixed-integer zero-one programming problems. *SIAM Journal on Discrete Mathematics*, 3:411–430.

[30] Szegedy, M. 1994. A note on the theta number of Lovász and the generalized Delsarte bound. *35th Annual Symposium on Foundations of Computer Science*, pages 36–39.