Copositivity cuts for improving SDP bounds on the clique number

Immanuel M. Bomze*
Florian Frommlet*
Marco Locatelli△

* ISDS, University of Vienna, Austria

△ DI, University of Turin, Italy

This version: November 13, 2008

Abstract

Adding cuts based on copositive matrices, we propose to improve Lovász' bound θ on the clique number and its tightening θ' introduced by McEliece, Rodemich, Rumsey, and Schrijver. Candidates for cheap and efficient copositivity cuts of this type are obtained from graphs with known clique number. The cost of recently established semidefinite programming bound hierarchies starting with θ' rapidly increases with the order (and quality requirements). By contrast, the bounds proposed here are relatively cheap in the sense that computational effort is comparable to that required for θ'.

Keywords: Lovász' Bound, Semidefinite Programming, Maximum Clique Problem.

1 Introduction

Consider a loopless undirected graph $\mathcal{G} = (V, \mathcal{E})$ with vertex set V (the order of $\mathcal{G}$ is $|V|$) and edge set $\mathcal{E}$. The *Maximum Clique Problem (MCP)* amounts at finding a complete subgraph of largest possible order in $\mathcal{G}$ [2], the so-called *clique number*, denoted by $\omega(\mathcal{G})$. Many upper bounds have been proposed for $\omega(G)$. Some of them are based on the solution of a *semidefinite program* (SDP), including the well known θ' bound [16], [18], an improvement of Lovász' bound θ [15] which is sometimes called LoMERoRuS bound to account for all authors involved. Our aim in this paper is to propose improvements of this bound which can be computed with comparable effort to that required for θ'. This distinction is important since refinements of the θ' bound based on hierarchies of semidefinite bounds (see [8, 10, 12, 13, 17]) and some dominance results for bounds in the hierarchies over those proposed in this paper will be proved below. On the other hand, as we move up in the hierarchy, the computation of these bounds becomes more and more costly. Our approach improves upon θ' and, at the same time, keeps the cost of the improvement as low as possible.

Here we follow the cutting-plane idea well-known in Combinatorial Optimization: first we solve a SDP relaxation of the MCP, then we introduce one or more cuts violated by the solution of the relaxation, to tighten the bound. Our novel contribution consists in specifying (a) the class of cuts which will be employed; and (b) the techniques to select appropriate cuts within this class. More precisely, in Section 2 we will briefly recall the θ' bound for MCP, and introduce a new class of copositivity cuts. Section 3 deals with other recently developed refinements of the θ' bound, including triangle inequalities [9], and the different hierarchies presented in [8], [12, 13], and [17]. In Section 4 we will present some theoretical results describing the behaviour of θ' and copositivity cut improvements under constructions like cosums and products of graphs. These findings will motivate the heuristics put forth in the subsequent sections. In Section 5 we will provide criteria to drive the choice of a cut and we will propose techniques to select good cuts with respect to the given criteria; finally, in Section 6 we will report preliminary computational experiences. These show that the approach is promising, yet there may be need of further improvement.

In the sequel, we employ the following notation: $\mathbb{R}^n_+$ is the positive orthant of n-dimensional Euclidean space $\mathbb{R}^n$, while I_n is the $n \times n$ identity matrix, $E_n = uu^\top$ the all-ones $n \times n$ matrix, and $u = [1, \ldots, 1]^\top \in \mathbb{R}^n$ with $^\top$ denoting transposition. Let $\mathcal{S}^n$ denote the set of all *symmetric* $n \times n$ matrices. Then the cone of *copositive matrices* $\mathcal{C}^n$ is defined as

$$\mathcal{C}^n = \{C \in \mathcal{S}^n : x^\top C x \geq 0 \quad \text{for all } x \in \mathbb{R}^n_+\}\,.$$

Due to $x^\top C x = \text{trace}\,(C x x^\top)$, the dual cone of $\mathcal{C}^n$ is

$$[\mathcal{C}^n]^* = \text{ conv } \left\{ x x^\top : x \in \mathbb{R}^n_+ \right\}\,,$$

the cone of *completely positive matrices*. $\mathcal{P}^n \subset \mathcal{C}^n$ denotes the cone of *positive-semidefinite* (psd) matrices, and $\mathcal{N}^n \subset \mathcal{C}^n$ the cone of symmetric matrices with no negative entries. Given $\{A, B\} \subset \mathcal{S}^n$, we will write $A \succeq B$ to signify $A - B \in \mathcal{P}^n$, and $A \geq B$ if $A - B \in \mathcal{N}^n$. The Frobenius inner product for such matrices is denoted by $A \bullet B := \text{trace}\,(AB)$.

For a set V and an integer $r \geq 0$, denote by $\binom{V}{r} = \{A \subseteq V : |A| = r\}$. Thus, a loopless undirected graph is given by $\mathcal{G} = (V, \mathcal{E})$ with $\mathcal{E} \subseteq \binom{V}{2}$. Its complement is denoted by $\overline{\mathcal{G}} = (V, \binom{V}{2} \setminus \mathcal{E})$. In the sequel, we consider two types of induced subgraphs $\mathcal{G}' = (V', \mathcal{E}')$: a *vertex-induced subgraph* with $V' \subset V$ and $\mathcal{E}' = \mathcal{E} \cap \binom{V'}{2}$, and the *edge-induced subgraph* where all vertices and some edges are kept: $V' = V$ but $\mathcal{E}' \subset \mathcal{E}$. Following the standard terminology, we call the latter also a *spanning subgraph* of $\mathcal{G}$.

2 Copositivity cuts tighten θ'

2.1 SDP bounds and copositivity cuts

We first recall some results about the upper bound $\theta'(\mathcal{G})$ for the clique number $\omega(\mathcal{G})$ of a graph $\mathcal{G}$ of order $n = |V|$. Let $A_\mathcal{G} \in \mathcal{S}^n$ be its adjacency matrix and

$$Q_\mathcal{G} = E_n - A_\mathcal{G} = I_n + A_{\overline{\mathcal{G}}}$$

with $A_{\overline{\mathcal{G}}}$ the adjacency matrix of the complementary graph. Then the MCP can be formulated as a copositive program [1, 7], e.g., in the form given by [8]:

$$\omega(\mathcal{G}) = \min\{t \in \mathbb{R} : t\,Q_\mathcal{G} - E_n \in \mathcal{C}^n\}\,. \tag{1}$$

Replacing the copositive cone $\mathcal{C}^n$ by the (zero-order) approximation $\mathcal{K}^n_0 = \mathcal{P}^n + \mathcal{N}^n \subset \mathcal{C}^n$ in (1) leads to the relaxation

$$\theta'(\mathcal{G}) = \min\left\{t \in \mathbb{R} : t\,Q_\mathcal{G} - E_n \in \mathcal{K}^n_0\right\}\,. \tag{2}$$

$\theta'(\mathcal{G})$ is the (LoMERoRuS) [16, 18] tightening of the Lovász bound [15] usually denoted by $\theta(\mathcal{G})$. The larger bound $\theta(\mathcal{G})$ results if $\mathcal{K}^n_0 = \mathcal{P}^n + \mathcal{N}^n$ is simply replaced by its subset $\mathcal{P}^n$ in (2).

For (2) strong duality holds, and the dual problem is given by

$$\theta'(\mathcal{G}) = \max\left\{E_n \bullet X : Q_{\mathcal{G}} \bullet X = 1\,,\; X \in \mathcal{P}^n \cap \mathcal{N}^n\right\}\,. \tag{3}$$

But, as pointed out in [8], a more frequently used SDP formulation of $\theta'(\mathcal{G})$ which only seemingly is stronger than (3) is

$$\theta'(\mathcal{G}) = \max\left\{E_n \bullet X : I_n \bullet X = 1\,,\; A_{\overline{\mathcal{G}}} \bullet X = 0\,,\; X \in \mathcal{P}^n \cap \mathcal{N}^n\right\}\,. \tag{4}$$

We note that the support of an optimal solution $X^\star$ of (4) is a subset of the support of $A_{\mathcal{G}} + I_n$, i.e., $X^\star_{ij} = 0$ whenever $\{i,j\} \notin \mathcal{E}$ and $i \neq j$. This observation is important for constructing promising cuts.

In [4] it has been proposed to improve the copositive bound for the general quadratic form $x^\top Q x$ over the unit simplex $\Delta = \{x \in \mathbb{R}^n_+ : \sum_j x_j = 1\}$ by means of additional cuts. If we imitate this approach for a general copositive program of the form (which covers all mixed-binary quadratic programs [6])

$$\max\left\{C \bullet X : \mathcal{A}(X) = b\,,\; X \in [\mathcal{C}^n]^*\right\}\,, \tag{5}$$

we consider a finite set of nontrivial copositive matrices $\{C_1, \ldots, C_s\} \not\ni O$, and the generated cone

$$\mathcal{D} := \left\{\sum_{j=1}^{s} y_j C_j : y \in \mathbb{R}^s_+\right\} \subset \mathcal{C}^n\,, \tag{6}$$

which satisfies $\mathcal{K}^n_0 + \mathcal{D} \subset \mathcal{C}^n$ by convexity of $\mathcal{C}^n$. In dual terms, we have $[\mathcal{C}^n]^* \subset [\mathcal{K}^n_0]^* \cap \mathcal{D}^* = \mathcal{P}^n \cap \mathcal{N}^n \cap \mathcal{D}^*$, so we relax (5) to

$$\max\left\{C \bullet X : \mathcal{A}(X) = b\,,\; C_j \bullet X \geq 0 \;\forall j\,,\; X \in \mathcal{P}^n \cap \mathcal{N}^n\right\}\,, \tag{7}$$

since the feasible set of (5) is contained in that of (7) which is an SDP. Returning to our problem to tighten $\theta'(\mathcal{G})$, we specialize $C = E_n$ and $\mathcal{A}(X) = Q_{\mathcal{G}} \bullet X$ as well as $b = 1$, to arrive at

$$\theta^{\mathcal{D}}(\mathcal{G}) := \max\left\{E_n \bullet X : Q_{\mathcal{G}} \bullet X = 1\,,\; C_j \bullet X \geq 0 \;\forall j\,,\; X \in \mathcal{P}^n \cap \mathcal{N}^n\right\}\,, \tag{8}$$

with its dual

$$\theta^{\mathcal{D}}(\mathcal{G}) = \min\left\{t \in \mathbb{R} : t\, Q_{\mathcal{G}} - E_n \in \mathcal{K}^n_0 + \mathcal{D}\right\}\,. \tag{9}$$

Note that strong duality holds since both (9) and (8) are strictly feasible; e.g., $X = \frac{1}{Q_{\mathcal{G}} \bullet (I_n + E_n)}(I_n + E_n) \in \mathcal{P}^n \cap \mathcal{N}^n$ satisfies Slater's condition

$$C_j \bullet X = \frac{1}{Q_{\mathcal{G}} \bullet (I_n + E_n)}[\mathrm{trace}\,(C_j) + E_n \bullet C_j] \;>\; 0 \quad \text{since } C_j \neq O\,.$$

Therefore, our idea is to employ copositive matrices C_j to define linear cuts for obtaining a tighter bound $\theta^{\mathcal{D}}(\mathcal{G})$. Below now we deal with the question *how to select these copositive matrices.*

2.2 Finding efficient copositivity cuts

The basic idea to construct candidates of copositive matrices relies on the copositive formulation of the MCP, seen from the reverse side. Let $\mathcal{H} = (V', \mathcal{E}')$ of order $|V'| = m \le n$ be a graph of known clique number $\omega(\mathcal{H})$. Without loss of generality, we may and do assume that $\mathcal{H}$ is a spanning subgraph of a vertex-induced subgraph of $\mathcal{G}$, i.e., that $V' \subseteq V$.

Then it follows immediately from (1) that $C'_{\mathcal{H}} = \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E_m - A_{\mathcal{H}} \in \mathcal{C}^m$, so that this matrix can be used for a *copositivity cut* based on

$$C_{\mathcal{H}} = \begin{pmatrix} C'_{\mathcal{H}} & O \\ O & O \end{pmatrix} \in \mathcal{C}^n . \tag{10}$$

For any $X \in \mathcal{P}^n \cap \mathcal{N}^n$, denote by $X' = [X_{ij}]_{i,j \in V'} \in \mathcal{P}^m \cap \mathcal{N}^m$ the restriction of X to $V' \times V'$. Then we have

$$C_{\mathcal{H}} \bullet X = C'_{\mathcal{H}} \bullet X' = \left(1 - \tfrac{1}{\omega(\mathcal{H})}\right) E_m \bullet X' - A_{\mathcal{H}} \bullet X' ,$$

and the additional inequality constraint in (8) with $s = 1$ can be written as

$$A_{\mathcal{H}} \bullet X' \le \left(1 - \tfrac{1}{\omega(\mathcal{H})}\right) E_m \bullet X' . \tag{11}$$

We will denote bounds obtained by this kind of copositivity cuts obtained via (8) and (10) as

$$\theta^{\mathcal{H}}(\mathcal{G}) := \theta^{\mathcal{D}}(\mathcal{G}) \quad \text{with} \quad \mathcal{D} = \mathbb{R}_+ C_{\mathcal{H}} . \tag{12}$$

Suppose we have obtained a solution $X^\star$ of (3). Now, to strictly improve $\theta'(\mathcal{G})$ by $\theta^{\mathcal{H}}(\mathcal{G})$ we search for candidate graphs $\mathcal{H}$ with known clique number for which $X^\star$ violates inequality (11). So we have to look for some graph $\mathcal{H}$ with *known* clique number $\omega(\mathcal{H})$ such that the quantity

$$f(\mathcal{H}) = -\left(1 - \frac{1}{\omega(\mathcal{H})}\right) E_m \bullet (X^\star)' + A_{\mathcal{H}} \bullet (X^\star)' \tag{13}$$

is positive.

Of course, the set of candidates $\mathcal{H}$ should be restricted to "sufficiently easy" graphs, namely with $\omega(\mathcal{H})$ either computable by very little effort or known beforehand. In particular, we concentrated on triangle-free graphs (TFG, with clique number 2) and on K_4-free graphs (K_4-FG, with clique number 3). Before discussing in Section 5 below how to detect candidates satisfying $f(\mathcal{H}) > 0$, in the following two sections we first investigate relations between various other bounds from the literature and copositivity cut bounds, and then we present a couple of theoretical results.

3 Comparison with other bounds

Recently Dukanović and Rendl in [9] used cuts for the following strengthening of θ':

$$\begin{aligned}\theta^{-\triangle}(\mathcal{G}) \;&=\; \max\big\{E_n \bullet X : I_n \bullet X = 1\,,\; A_{\overline{\mathcal{G}}} \bullet X = 0\,,\; X \in \mathcal{P}^n \cap \mathcal{N}^n\,,\\ &\quad X_{ij} \le X_{ii}\,,\;\; X_{ik} + X_{jk} \le X_{ij} + X_{kk}\,,\; \text{all } \{i,j,k\} \subseteq V\big\}\,. \qquad (14)\end{aligned}$$

This is the SDP formulation (4) supplemented with triangle inequalities, adding $\mathcal{O}(n^3)$ cuts $C \bullet X \ge 0$ with matrices C containing the principal block

$$\begin{pmatrix} 2 & -1 \\ -1 & 0 \end{pmatrix}.$$

As this matrix is not copositive, (14) cannot be seen as a special case of (8). So we suspect that $\theta^{-\triangle}(\mathcal{G})$ is not comparable to $\theta^{\mathcal{H}}(\mathcal{G})$ in general, although the comparison figures in Subsection 6.1 indicate a slight advantage of the copositivity cut bound, but this may be also traced back to the larger amount of time dedicated to find cuts. For future research it may be interesting to combine triangle inequalities with the cuts proposed in this paper.

Different hierarchies of SDP bounds were proposed in [8] and [17], for which θ' is the zero-order approximation. In [8] the bounds

$$\vartheta^{(r)}(\mathcal{G}) = \min\{t : tQ_{\mathcal{G}} - E_n \in \mathcal{K}_r^n\}, \quad r = 0, 1, \ldots \qquad (15)$$

have been studied. The matrix cones $\mathcal{K}_r^n$ are approximations of the copositive cone $\mathcal{C}^n$ which become tighter with increasing r. Therefore, while for $r = 0$ we have the usual θ' bound, as r increases we get tighter bounds. On the other hand the cost of computing the bounds increases with r. Indeed, solving (15) requires the solution of an SDP with matrix variables of size $n^{r+1} \times n^{r+1}$. In [17] the following variant of (15) has been proposed:

$$\nu^{(r)}(\mathcal{G}) = \min\{t : tQ_{\mathcal{G}} - E_n \in \mathcal{Q}_r^n\}, \quad r = 0, 1, \ldots, \qquad (16)$$

where $\mathcal{Q}_r^n$ are suitably defined subcones of $\mathcal{K}_r^n$ for all r and hence $\nu^{(r)}(\mathcal{G}) \ge \vartheta^{(r)}(\mathcal{G})$. Like $\mathcal{K}_r^n \subset \mathcal{K}_{r+1}^n \subset \mathcal{C}_r^n$, also this series of cones are increasing with increasing r, i.e., $\mathcal{Q}_r^n \subset \mathcal{Q}_{r+1}^n$, while $\mathcal{Q}_0^n = \mathcal{K}_0^n$.

Finally, we shortly address Lasserre's hierarchy of bounds [12, 13], defined as

$$\begin{aligned}\lambda^{(r)}(\mathcal{G}) \;&= \max\{ \sum_{i\in V} x_{\{i\}} : \;\; x_\emptyset = 1\,,\; x_e = 0\,,\; \text{all } e \in \tbinom{V}{2} \setminus \mathcal{E}\,,\\ &\qquad x_S \ge 0\,, \text{all } S \in \tbinom{V}{r+2}\,;\; M_r(x) \succeq 0\}\,,\end{aligned} \qquad (17)$$

where for a vector $(x_I)_I$ indexed by all subsets of V, the *(combinatorial) moment matrix* $M_r(x)$ of order r, with $\sum_{k=0}^{r+1}\binom{n}{k} = \mathcal{O}(n^{r+1})$ rows and columns, is given by its (I,J)-th entry $x_{I\cup J}$ for all $I \subseteq V$ and $J \subseteq V$ containing not more than $r+1$ elements. Again, an $n^{r+1} \times n^{r+1}$ matrix variable is involved in (17). As $M_r(x)$ is a principal submatrix of $M_{r+1}(x)$, we clearly have $\lambda^{(r)}(\mathcal{G}) \geq \lambda^{(r+1)}(\mathcal{G}) \geq \omega(\mathcal{G})$. The last inequality follows because the characteristic vector of any clique C (with I-th entry equal to unity if $I \subseteq C$, zero otherwise) is feasible to (17) with objective $|C|$. It holds that $\lambda^{(0)}(\mathcal{G}) = \theta'(\mathcal{G})$, as in the hierarchies previously mentioned where we also have $\nu^{(0)}(\mathcal{G}) = \vartheta^{(0)}(\mathcal{G}) = \theta'(\mathcal{G})$. Further, it is shown in [13] that $\omega(\mathcal{H}) = \lambda^{(r)}(\mathcal{H})$ if $\omega(\mathcal{H}) \leq r+1$.

The following result relates copositivity cut bounds obtained by graphs with clique number not larger than $r+1$ with $\nu^{(r)}(\mathcal{G})$ for $r \leq 5$, and with $\vartheta^{(r)}(\mathcal{G})$ or $\lambda^{(r)}(\mathcal{G})$, for $r \leq 7$.

Theorem 3.1 *The best bound which can be obtained by the introduction of any number of cuts based on graphs with clique number not larger than* $r+1$ *in (8) can not be tighter than* $\nu^{(r)}(\mathcal{G})$ *for* $r \leq 5$ *and not tighter than* $\vartheta^{(r)}(\mathcal{G})$ *or* $\lambda^{(r)}(\mathcal{G})$ *for* $r \leq 7$.

Proof. Suppose we cut with m graphs $\mathcal{H}_j$ with known $\omega_j = \omega(\mathcal{H}_j) \leq r+1$ for $r \leq 5$, all $1 \leq j \leq m$. Corollary 7 in [17] states that $\nu^{(r)}(\mathcal{H}_j) = \omega_j$. Then we have by (16) that $\omega_j(E_n - A_{\mathcal{H}_j}) - E_n \in \mathcal{Q}_r^n$ or, equivalently:

$$C_j = \left(1 - \tfrac{1}{\omega_j}\right) E_n - A_{\mathcal{H}_j} \in \mathcal{Q}_r^n\,, \quad \text{all } 1 \leq j \leq m\,.$$

Consequently, with $\mathcal{D}$ as in (6) we get $\mathcal{K}_0^n + \mathcal{D} \subseteq \mathcal{Q}_n^r$ and thus $\theta^{\mathcal{D}}(\mathcal{G}) \geq \nu^{(r)}(\mathcal{G})$. A similar argument using [10, Corollary 1] yields the second assertion. Finally, in view of $\lambda^{(r)}(\mathcal{G}) \leq \vartheta^{(r)}(\mathcal{G})$ for any graph $\mathcal{G}$ and any $r \geq 0$ as stated in [10, Theorem 4], it immediately follows from the preceding arguments that the best bound obtained by introduction of any number of cuts based on graphs with clique number not larger than $r+1$ in (8) can not be tighter than $\lambda^{(r)}(\mathcal{G})$ for $r \leq 7$. □

Of course, the $\vartheta^{(r)}(\mathcal{G})$ – and similarly the bounds $\nu^{(r)}(\mathcal{G})$ and $\lambda^{(r)}(\mathcal{G})$ – are much more expensive to compute than our bounds, because there $n^{r+1} \times n^{r+1}$ matrix variables (or a comparable number of $n \times n$ matrices) are used, while we use only very few $n \times n$ matrix variables. The rapid increase of the size of the SDPs involved as r increases is reflected, e.g. by [17, p.18] where it is stated that computation of $\nu^{(4)}(\overline{G_{17}})$ is already beyond the current computational capabilities, where G_{17} is a special graph with 17 nodes (see also Subsection 6.1).

Relations between bounds obtained by adding copositivity cuts with clique number not larger than $r+1$ and the bounds (15) and (16), respectively, for $r \geq 8$ and $r \geq 6$ are at the moment not clear, although Conjecture 5.1 in [8] (proved for r up to 7 in [10]) suggests that for all $r \geq 2$, bound $\vartheta^{(r)}(\mathcal{G})$ dominates all bounds obtained by the introduction of cuts based on graphs with clique number not larger than $r+1$.

The result stated in Theorem 3.1 can not be extended to cuts based on graphs with clique number larger than $r+1$. A trivial example of this fact is represented by graph $\overline{G_8}$ from [17]. For this graph it holds that $\nu^{(1)}(G_8) = 3.04328$ while cutting with K_4-free graphs trivially delivers the exact clique number since $\overline{G_8}$ itself is K_4-free. See Subsection 6.1 below for more detailed evidence.

4 Two theoretical results

In this section we present a couple of theoretical results. The first one establishes that we can have arbitrarily large improvements over θ' even when cutting with subgraphs with a fixed clique number. The second one shows that for graphs of special structure (cosum of smaller graphs), we can derive bounds equal to the sum of the bounds for their components.

4.1 Arbitrarily large gap with respect to θ'

First we show that once we have a *single* graph for which the bound obtained by adding a cut is exact, then we are able to find an infinite class of graphs with arbitrarily large clique numbers for which we are able to get an exact bound after adding a copositivity cut.

In order to define the *direct* or *strong product* $*$ between two graphs $\mathcal{G}_1$ and $\mathcal{G}_2$ of order n_1 and n_2, respectively, via their adjacency matrices, recall that the Kronecker product $\otimes$ transforms any two symmetric binary matrices of order n_i ($i = 1, 2$) into a symmetric binary $n \times n$ matrix with $n = n_1 n_2$. Then the direct product is defined as follows:

$$A_{\mathcal{G}_1 * \mathcal{G}_2} := I_{n_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes I_{n_2} + A_{\mathcal{G}_1} \otimes A_{\mathcal{G}_2} \, , \qquad (18)$$

or, equivalently

$$I_n + A_{\mathcal{G}_1 * \mathcal{G}_2} = (I_{n_1} + A_{\mathcal{G}_1}) \otimes (I_{n_2} + A_{\mathcal{G}_2}) \, , \qquad (19)$$

which is the same as

$$Q_{\overline{\mathcal{G}_1 * \mathcal{G}_2}} = Q_{\overline{\mathcal{G}_1}} \otimes Q_{\overline{\mathcal{G}_2}} \,. \tag{20}$$

While for the direct product both graph parameters θ and ω are multiplicative [11], this does not seem to hold in general for the θ' bound. However, [3, Theorem 4.3] states sufficient conditions which imply

$$\theta'(\mathcal{G}_1 * \mathcal{G}_2) = \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) \,. \tag{21}$$

For instance, if one factor $\mathcal{G}_1 = K_n$ is the complete graph with n vertices, then (21) holds.

The following theorem gives a whole class of graphs with arbitrarily large clique numbers for which copositivity cuts yield exact bounds, starting from a single graph for which a copositivity cut is tight.

Theorem 4.1 *Assume that $\theta'(\mathcal{G}) > \omega(\mathcal{G}) = \theta^{\mathcal{H}}(\mathcal{G})$ for a graph of order m, where $\mathcal{H}$ is a spanning subgraph of $\mathcal{G}$ with clique number $\omega(\mathcal{H})$. Consider the product $\mathcal{G}_n = K_n * \mathcal{G}$ and the spanning subgraph $\mathcal{H}_n$ of $\mathcal{G}_n$ with adjacency matrix $A_{\mathcal{H}_n} = E_n \otimes A_{\mathcal{H}}$ (note that, by (18), $\mathcal{H}_n$ is sparser than $K_n * \mathcal{H}$).*

Then $\omega(\mathcal{H}_n) = \omega(\mathcal{H}) \leq m$ and

$$\theta^{\mathcal{H}_n}(\mathcal{G}_n) = n\omega(\mathcal{G}) = \omega(\mathcal{G}_n) \quad \textit{for all } n \,.$$

Proof. Abbreviate by $\omega^\star = \omega(\mathcal{G})$. The clique number for $K_n * \mathcal{G}$ is equal to $n\omega^\star$. Then, in order to prove that the addition of cut $\mathcal{H}_n$ leads to the exact bound we need to show that with $Q_n = Q_{\mathcal{G}_n} = E_{mn} - A_{\mathcal{G}_n}$ and $C_n = \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E_{mn} - A_{\mathcal{H}_n} \in \mathcal{C}^{mn}$, we get

$$n\omega^\star Q_n - E_{mn} - \alpha C_n \in \mathcal{K}_0^{mn}$$

for some $\alpha \geq 0$. Now by construction and in view of (19) which gives $I_{mn} + A_{\mathcal{G}_n} = E_n \otimes (I_m + A_{\mathcal{G}})$, we have

$$\begin{aligned} Q_n &= E_{mn} + I_{mn} - (I_{mn} + A_{\mathcal{G}_n}) = E_{mn} + I_{mn} - E_n \otimes (I_m + A_{\mathcal{G}}) \\ &= E_n \otimes Q_{\mathcal{G}} + (I_n - E_n) \otimes I_m \,. \end{aligned} \tag{22}$$

By assumption, we have for $C_{\mathcal{H}} = \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E_m - A_{\mathcal{H}} \in \mathcal{C}^m$ that

$$\omega^\star Q_{\mathcal{G}} = E_m + \beta C_{\mathcal{H}} + N_m + P_m, \tag{23}$$

for some $N_m \in \mathcal{N}^m$, $P_m \in \mathcal{P}^m$, and $\beta > 0$ (note that $\theta'(\mathcal{G}) > \omega(\mathcal{G})$ implies strict inequality). Further it is immediate that $C_n = E_n \otimes C_{\mathcal{H}}$ for all n.

From (22) and (23) we deduce, after some rearrangements and noting that $Q_{\mathcal{G}} - I_m = A_{\overline{\mathcal{G}}}$ is also a binary matrix,

$$\begin{aligned} n\omega^\star Q_n &= nE_n \otimes (\omega^\star Q_{\mathcal{G}}) + n\omega^\star (I_n - E_n) \otimes I_m \\ &= (n-1)\omega^\star E_n \otimes (Q_{\mathcal{G}} - I_m) + E_n \otimes (\omega^\star Q_{\mathcal{G}}) + \\ &\quad + \omega^\star (nI_n - E_n) \otimes I_m \\ &= (n-1)\omega^\star E_n \otimes A_{\overline{\mathcal{G}}} + E_n \otimes (E_m + \beta C_{\mathcal{H}} + N_m + P_m) + \\ &\quad + \omega^\star (nI_n - E_n) \otimes I_m \\ &= (n-1)\omega^\star E_n \otimes A_{\overline{\mathcal{G}}} + E_{mn} + \beta C_n + E_n \otimes N_m + \\ &\quad + E_n \otimes P_m + \omega^\star (nI_n - E_n) \otimes I_m \\ &= E_{mn} + \beta C_n + E_n \otimes M_m + [E_n \otimes P_m + \omega^\star (nI_n - E_n) \otimes I_m] \ , \end{aligned} \tag{24}$$

where the matrix $M_m = (n-1)\omega^\star A_{\overline{\mathcal{G}}} + N_m$ has no negative entries. Since $E_n \otimes P_m + \omega^\star (nI_n - E_n) \otimes I_m \succeq O$ as the sum of two psd. matrices (recall that Kronecker products of psd. factors are again psd.), this concludes the proof, putting $\alpha = \beta$. □

An easy application of the above theorem is the following. It is well known that the 5-cycle C_5 is the smallest graph for which $\theta'(\mathcal{G}) > \omega(\mathcal{G})$, with $\theta'(C_5) = \theta(C_5) = \sqrt{5}$, and $\omega(C_5) = 2$. Now let us define $\mathcal{G}_n := K_n * C_5$. Relation (21) shows that $\theta'(\mathcal{G}_n) = n\sqrt{5}$, while $\omega(\mathcal{G}_n) = 2n$, so the gap between the θ' bound and the clique number becomes arbitrarily large with growing n. Now we define $A_{\mathcal{H}_n} := E_n \otimes A_{C_5}$. Then the graph $\mathcal{H}_n$ is a triangle-free spanning subgraph of $\mathcal{G}_n$ and Theorem 4.1 shows that using it leads to the exact bound $2n$.

4.2 Cosums of graphs

Other classes of graphs for which we can make the gap between θ' and the bound obtained by adding cuts large, can be obtained by introducing graph *cosums.* The (direct) sum of two graphs $\mathcal{G}_1 = (V_1, \mathcal{E}_1)$ and $\mathcal{G}_2 = (V_2, \mathcal{E}_2)$ with disjoint vertex sets V_i of order n_i is simply the graph $\mathcal{G} = (V_1 \cup V_2, \mathcal{E}_1 \cup \mathcal{E}_2)$. This means no edges are added to the disjoint union, in terms of adjacency matrices

$$A_{\mathcal{G}} = \begin{bmatrix} A_{\mathcal{G}_1} & O \\ O & A_{\mathcal{G}_2} \end{bmatrix} .$$

As we are dealing with cliques rather than stable sets, in the sequel we will employ the cosum of two such graphs $\mathcal{G}_i$, denoted by $\mathcal{G}_1 \oplus \mathcal{G}_2$, which is the complement of the sum of the complements of $\mathcal{G}_1$ and $\mathcal{G}_2$. Again, the vertex set here is $V_1 \cup V_2$, but now e is an edge in $\mathcal{G}_1 \oplus \mathcal{G}_2$ either if it is an edge of one of the graphs or if it joins vertices from different vertex sets. Abbreviating $Q_i = Q_{\mathcal{G}_i}$, we thus have for the cosum $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$ that

$$E_n - A_{\mathcal{G}} = Q_{\mathcal{G}} = \begin{bmatrix} Q_1 & O \\ O & Q_2 \end{bmatrix} . \tag{25}$$

Obviously, a vertex subset S with $S_i = S \cap V_i$ is a clique in $\mathcal{G}_1 \oplus \mathcal{G}_2$ if and only if S_i are cliques in $\mathcal{G}_i$, so that $\omega(\mathcal{G}_1 \oplus \mathcal{G}_2) = \omega(\mathcal{G}_1) + \omega(\mathcal{G}_2)$. The result in [3, Theorem 4.1] establishes the same additivity property for θ':

$$\theta'(\mathcal{G}_1 \oplus \mathcal{G}_2) = \theta'(\mathcal{G}_1) + \theta'(\mathcal{G}_2) . \tag{26}$$

Now, let us consider two graphs $\mathcal{G}_1$ and $\mathcal{G}_2$, respectively of order n_1 and n_2. Next we consider the cosum $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$ of order $n = n_1 + n_2$. We also assume that $\mathcal{H}_1$ and $\mathcal{H}_2$ are two spanning subgraphs of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively, with known clique numbers $\overline{\omega}_i = \omega(\mathcal{H}_i)$. Then $C_i = \left(1 - \frac{1}{\overline{\omega}_i}\right) E - A_{\mathcal{H}_i}$ are copositive. Let $\mathcal{D}_i = \mathbb{R}_+ C_i$ and $\theta^{\mathcal{D}_i}(\mathcal{G}_i)$ be the bounds obtained by using the cuts based on the spanning subgraphs $\mathcal{H}_i$. We recall that in [4, Section 7.4] decompositions of the following form are considered:

$$Q_i = P_i + N_i + \alpha_i C_i , \tag{27}$$

where $P_i \in \mathcal{P}^{n_i}$ while $N_i \in \mathcal{N}^{n_i}$ with diag $(N_i) = o$, and $\alpha_i \geq 0$. It was proved that there exists an *optimal* decomposition $P_i^\star \in \mathcal{P}^{n_i}$, $N_i^\star \in \mathcal{N}^{n_i}$ and $\alpha_i^\star \geq 0$ such that

$$Q_i = P_i^\star + N_i^\star + \alpha_i^\star C_i . \tag{28}$$

"Optimal" means here that $\min_{x \in \Delta} x^\top P_i^\star x$ is the largest among all possible decompositions of the type (27), and moreover we have

$$\ell^{\mathcal{D}_i}(\mathcal{G}_i) := \frac{1}{\theta^{\mathcal{D}_i}(\mathcal{G}_i)} = \pi_i^\star = \min_{x \in \Delta} x^\top P_i^\star x . \tag{29}$$

This follows from an elementary property concerning swapping objective and a single constraint in a linear program over a cone $\mathcal{K}$:

$$\max \{C \bullet X : Q \bullet X = 1 , X \in \mathcal{K}\} = 1/ \min \{Q \bullet Y : C \bullet Y = 1 , Y \in \mathcal{K}\} ,$$

provided both functionals $Q \bullet X$ and $C \bullet X$ are strictly positive over $\mathcal{K} \setminus \{O\}$. Applied to our set-up with $\mathcal{K} = [\mathcal{K}_0^n + \mathcal{D}]^* = \{Y \in \mathcal{P}^n \cap \mathcal{N}^n : C_j \bullet Y \geq 0 \, \forall j\}$, this yields now indeed via (8)

$$\ell^{\mathcal{D}_i}(\mathcal{G}_i) = \min \{Q_{\mathcal{G}_i} \bullet Y : E_{n_i} \bullet Y = 1, Y \in \mathcal{K}\} .$$

The latter is the relaxation of $\min_{x\in\Delta} x^\top Q x$ leading to $\min_{x\in\Delta} x^\top P_i^\star x$, as detailed in [4, Section 6.2 and 7.4].

Now let

$$C = \begin{bmatrix} \alpha_1^\star C_1 & O \\ O & \alpha_2^\star C_2 \end{bmatrix} \in \mathcal{C}^n \quad \text{and} \quad \mathcal{D} = \mathbb{R}_+ C\,. \tag{30}$$

Observe that the following result can be easily extended to the cosum of any number $k \geq 2$ of graphs.

Theorem 4.2 *The bound $\theta^{\mathcal{D}}(\mathcal{G})$ is equal to $\theta^{\mathcal{D}_1}(\mathcal{G}_1)+\theta^{\mathcal{D}_2}(\mathcal{G}_2)$. In particular, if the bounds $\theta^{\mathcal{D}_i}(\mathcal{G}_i)$ are exact, i.e. equal to $\omega(\mathcal{G}_i)$, then also bound $\theta^{\mathcal{D}}(\mathcal{G})$ is exact.*

Proof. What we need to prove is that

$$l^{\mathcal{D}}(\mathcal{G}) = \frac{\pi_1^\star \pi_2^\star}{\pi_1^\star + \pi_2^\star}.$$

Indeed, in such case it follows from (29) that

$$\theta^{\mathcal{D}}(\mathcal{G}) = \frac{1}{l^{\mathcal{D}}(\mathcal{G})} = \frac{1}{\pi_1^\star} + \frac{1}{\pi_2^\star} = \theta^{\mathcal{D}_1}(\mathcal{G}_1) + \theta^{\mathcal{D}_2}(\mathcal{G}_2)\,.$$

Again following [4, Section 7.4], we need to find the best possible among these decompositions:

$$E_n - A_{\mathcal{G}} = P + N + \alpha C,\ \ P \in \mathcal{P}^n,\ \ N \in \mathcal{N}^n \text{ with } \operatorname{diag}(N) = o\,,\ \alpha \geq 0\,, \tag{31}$$

i.e. the one for which $\min_{x\in\Delta} x^\top P x$ is as large as possible. Decompositions of type (31) for the matrix $Q_{\mathcal{G}} = E_n - A_{\mathcal{G}}$ are as follows by construction (25):

$$\begin{bmatrix} Q_1 & O \\ O & Q_2 \end{bmatrix} = \begin{bmatrix} P_1 & -Z \\ -Z & P_2 \end{bmatrix} + \begin{bmatrix} N_1 & Z \\ Z & N_2 \end{bmatrix} + \alpha \begin{bmatrix} \alpha_1^\star C_1 & O \\ O & \alpha_2^\star C_2 \end{bmatrix}, \tag{32}$$

where we must have that $Z \geq 0$, and necessarily

$$P_i + N_i + \alpha\alpha_i^\star C_i\,, \quad i = 1, 2\,,$$

are decompositions of type (27) for Q_i. First we note that the best bound is certainly obtained when $Z = O$. Indeed,

$$P = \begin{bmatrix} P_1 & -Z \\ -Z & P_2 \end{bmatrix} \in \mathcal{P}^n \quad \text{implies} \quad P_0 = \begin{bmatrix} P_1 & O \\ O & P_2 \end{bmatrix} \in \mathcal{P}^n$$

and $x^\top P x \leq x^\top P_0 x$ for all $x \in \mathbb{R}^n_+$, so the bound given by P_0 is at least as good as the one given by P. It immediately follows that the bound given by P_0 is obtained by solving the following simple one-dimensional problem

$$\min_{\lambda \in [0,1]} \quad \lambda^2 \pi_1 + (1-\lambda)^2 \pi_2 = \frac{\pi_1 \pi_2}{\pi_1 + \pi_2} \left(= \left[\pi_1^{-1} + \pi_2^{-1}\right]^{-1} \right)$$

with $\pi_i = \min_{x \in \Delta} x^\top P_i x > 0$. Thus, the best possible such bound is obtained if P_i and N_i are equal respectively to $P_i^\star$ and $N_i^\star$, i.e. the matrices appearing in the optimal decompositions (28) for Q_i, and if $\alpha = 1$. Then, the result on the cosum follows. □

After proving the result above, we need to point out a relevant fact. If we are aware of the cosum structure of a graph and we know its component graphs $\mathcal{G}_i$, then we do not even need the above result: indeed, what we can do is simply to compute a distinct bound for each component $\mathcal{G}_i$ and then sum up these bounds to derive a bound for $\mathcal{G}$. Therefore, here we are assuming that we are not aware of the cosum structure. In this case the result above, for which the explicit knowledge of the component graphs $\mathcal{G}_i$ is required, can not be employed in practice to derive the copositivity cut (30) but still proves the *existence* of such a cut and suggests that the proposed approach might work well for structured graphs like cosums, a fact which will be later confirmed by the computational experiments. Moreover, consider a graph $\mathcal{G}'$ obtained from the cosum graph $\mathcal{G}$ by removing edges connecting nodes in V_1 and V_2 in such a way that the clique number of $\mathcal{G}'$ is equal to that of $\mathcal{G}$. In this case decomposition (32) with $Z = O$, $P_i = P_i^\star$, $N_i = N_i^\star$, $i = 1, 2$, is not necessarily the optimal decomposition, but guarantees that bound $\theta^{\mathcal{D}}(\mathcal{G}')$ is not larger than $\theta^{\mathcal{D}_1}(\mathcal{G}_1) + \theta^{\mathcal{D}_2}(\mathcal{G}_2)$. In particular, equality holds if bounds $\theta^{\mathcal{D}_i}(\mathcal{G}_i)$, $i = 1, 2$, are exact.

5 Finding cuts: criteria and heuristics

While in the previous section we proved some theoretical results showing that adding copositivity cuts in some cases may lead to considerable improvements with respect to the θ' bound, we still need to define some practical approaches to choose a copositivity cut based on graphs with known clique number. We first need a criterion which drives the choice. A quite natural criterion to select a graph $\mathcal{H}$ defining a cut is to look for the one for which inequality (11) is most violated by the solution $X^\star$ of (3). Formally, for graphs $\mathcal{H}$ with a *fixed* clique number ω_0, we need to solve the following problem, recalling definition (13):

$$\max\{f(\mathcal{H}) : \omega(\mathcal{H}) = \omega_0\}. \tag{33}$$

Such a problem is in fact a combinatorial optimization problem. Actually, what we aim at is not merely to solve problem (33), but to detect different subgraphs $\mathcal{H}$ such that $f(\mathcal{H}) > 0$, because each of them corresponds to a valid cut. We will do that through a heuristic approach. Note that it is not our intention here to develop sophisticated strategies for detecting valid cuts. The approach proposed is rather based on simple ideas taken from the field of heuristics for combinatorial optimization problems, which can be certainly improved in a number of ways. All the same we would like to show that such a simple approach is already able to provide good valid cuts.

5.1 A decomposition heuristic

The proposed heuristic has the following input parameters

- k: the number of subsets V_r, $r = 1, \dots, k$, into which V is partitioned;
- for each $r \in \{1, \dots, k\}$, a value d_r (in the computations $d_r = 3$ or 4) ($d_r - 1$ will be the clique number of the subgraph we intend to build on the given subset of the partition).

We will later discuss how to choose these input parameters.
Given a node subset $V_r \subset V$ and the corresponding vertex-induced subgraph $\mathcal{G}_r$ with edge set

$$\mathcal{E}(V_r) = \{(i,j) \in \mathcal{E} \ : \ i, j \in V_r\} \, ,$$

in order to build a K_{d_r}-free subgraph over $\mathcal{G}_r$, we employ as a sub-procedure a greedy heuristic `Greedy`(V_r, A_r, d_r) which returns a K_{d_r}-free spanning subgraph $\mathcal{H}_r = (V_r, E_r)$ of $\mathcal{G}_r$, starting from a given subset of edges $A_r \subset \mathcal{E}(V_r)$ with $\omega(V_r, A_r) \leq d_r - 1$. This will be done by adding edges so that the f-value of the corresponding graph increases, and stopping when we can not add further edges without losing the property that the subgraph is K_{d_r}-free. To be more specific, we order edges $e = \{i, j\}$ such that their weights $w_e = X^\star_{ij}$ from the solution $X^\star$ of (3) are not increasing, and probe whether we can add them.

For a given partition $V_1, \dots, V_k$, with resulting subgraphs $\mathcal{H}_1, \dots, \mathcal{H}_k$, the corresponding value is given by the following objective function, to be maximized:

$$g(\mathcal{H}_1, \dots, \mathcal{H}_k) = \max_{r=1,\dots,k} f(\mathcal{H}_r) \, .$$

The heuristic attempts to improve the value of the current solution by swapping nodes between different members of the partition or by moving a node from one member to a different one, until there are no more changes which allow for an improvement.

A sensitive choice of k and of the d_r values should be related to θ'. If θ' is small, it makes sense to choose a small k (e.g., if graph $\mathcal{G}$ is already triangle-free we should even choose $k = 1$). For this reason we restricted our attention to combinations of d_r values equal to 3 or 4, $r = 1, \ldots, k$, such that

$$\lfloor \theta' \rfloor \leq \sum_{r=1}^{k} (d_r - 1) \leq \lfloor \theta' \rfloor + 20$$

In order to detect different valid cuts, we performed several runs of the heuristic with combinations of the d_r values satisfying the above condition. Note that each run of the heuristic returns at most a single valid cut, but the heuristic can be run arbitrarily often. The bound obtained by cutting simultaneously with all valid cuts is denoted by θ^{cop}. For the computational results in Section 6 we choose the number of runs such that the computation time to generate cuts was comparable with the time required by the solver `CSDP` [5] through `YALMIP` [14] to compute θ' for the corresponding graph. In summary the procedure to compute θ^{cop} takes roughly three times as long as computing θ'. We had also considered a faster version of the heuristic only allowing for combinations of d_r values satisfying the above condition and all equal to each other (all equal to 3 or all equal to 4). This gave in most cases a bound somewhere between θ' and θ^{cop} (results not shown).

For the sake of correctness it is important to point out here that the use of `CSDP` through `YALMIP` is not the most efficient one. Therefore, our claim above about the computation times of θ^{cop} should be reconsidered after a more efficient use of `CSDP`. On the other hand, we should also take into account that our current implementation of the proposed heuristic can very likely be improved, and, even more important, that other, more efficient heuristics could be defined in the future. In fact, in this paper our aim is to show that the proposed idea is promising, but we are aware that many improvements are still possible and actually hope that our work will stimulate future research and the development of more efficient strategies.

The details of the heuristic are as follows.

Decomposition heuristic

Initialization For each $i \in V$ select in a random way the subset V_r of the partition into which it will be inserted. For each $r \in \{1, \dots, k\}$, compute

$$\mathcal{H}_r = (V_r, A_r) = \texttt{Greedy}(V_r, \emptyset, d_r).$$

Step 1 For each $i \in V_r$, $j \in V_s$, $r \neq s$:

- set

$$V_r' = V_r \cup \{j\} \setminus \{i\}, \quad V_s' = V_s \cup \{i\} \setminus \{j\}, \quad V_t' = V_t \quad \text{for all} \quad t \neq r, s$$

- set

$$\begin{aligned} A_r' &= A_r \setminus \{(i,h) : \ h \in V_r, \ (i,h) \in A_r\}, \\ A_s' &= A_s \setminus \{(j,h) : \ h \in V_s, \ (j,h) \in A_s\}, \\ A_t' &= A_t \quad \text{for all} \quad t \neq r, s; \end{aligned}$$

- compute $\mathcal{H}_r' = (V_r', A_r'') = \texttt{Greedy}(V_r', A_r', d_r)$ and $\mathcal{H}_s' = (V_s', A_s'') = \texttt{Greedy}(V_s', A_s', d_s)$. Set $\mathcal{H}_t' = \mathcal{H}_t$ for all $t \neq r, s$.
- compute $g(\mathcal{H}_1', \dots, \mathcal{H}_k')$. If $g(\mathcal{H}_1', \dots, \mathcal{H}_k') > g(\mathcal{H}_1, \dots, \mathcal{H}_k)$, then go to Step 3, otherwise repeat Step 1 until there are no possible swaps (in this case go to Step 2)

Step 2 For each $i \in V_r$, $r \neq s$:

- Set

$$V_r' = V_r \setminus \{i\}, \quad V_s' = V_s \cup \{i\}, \quad V_t' = V_t \quad \text{for all} \quad t \neq r, s$$

- set

$$A_r' = A_r \setminus \{(i,h) : \ h \in V_r, \ (i,h) \in A_r\}, \quad A_t' = A_t \quad \text{for all} \quad t \neq r$$

- compute $\mathcal{H}_r' = (V_r', A_r'') = \texttt{Greedy}(V_r', A_r', d_r)$ and $\mathcal{H}_s' = (V_s', A_s'') = \texttt{Greedy}(V_s', A_s', d_s)$. Set $\mathcal{H}_t' = \mathcal{H}_t$ for all $t \neq r, s$.
- compute $g(\mathcal{H}_1', \dots, \mathcal{H}_k')$. If $g(\mathcal{H}_1', \dots, \mathcal{H}_k') > g(\mathcal{H}_1, \dots, \mathcal{H}_k)$, then go to Step 3, otherwise repeat Step 2 until there are no possible moves (in this case go to Step 4).

Step 3 Set

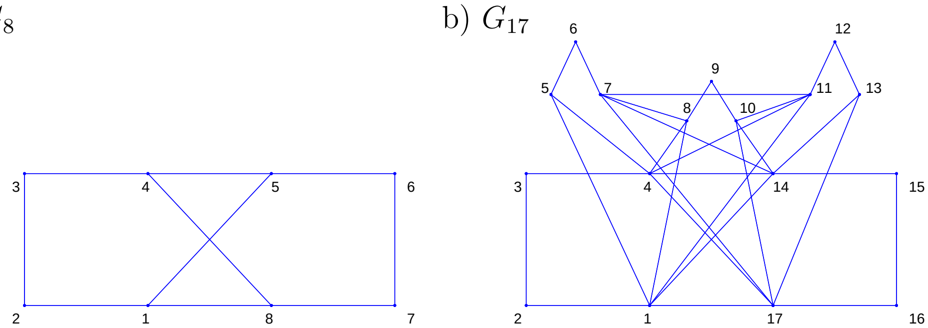
$$\mathcal{H}_t = \mathcal{H}_t' \quad \text{for all} \quad t \in \{1, \dots, k\}.$$

and go back to Step 1.

Step 4 None of the swaps and of the moves allows for an improvement and the algorithm stops.

Figure 1: Graphs introduced by Peña et al. [17]

a) G_8 b) G_{17}



6 Computational experience

First we illustrate our method by discussing computational results for some relatively small special graphs with the property that θ' is not exact even after truncation. Then we will show in Subsection 6.2 results for a wide class of structured graphs for which it is known that θ' bound is not exact. Finally we will present some results on random graphs in Subsection 6.3.

6.1 Some special small graphs

In a recent article, Peña and coworkers [17] consider the stability number of graphs, and investigate challenging graphs G_8, G_{11}, G_{14}, and G_{17}. For the clique number, we therefore have to look at the complement graphs $\overline{G_r}$, where $r \in \{8, 11, 14, 17\}$. For illustration, we depict G_8 and G_{17} in Figure 1 with a suitable vertex labelling.

The bounds obtained by our heuristic and by other methods for comparison are reported in Table 1. The graph $\overline{G_8}$ is K_4-free, so the heuristics of Section 5 with $k = 1$ and $d_1 = 4$ trivially leads to $\omega = 3$ itself. On the other hand, $\overline{G_8}$ is an example where there exists no cut based on triangle-free spanning subgraph that improves $\theta' = 3.4678$. For all four graphs $\theta^{\rm cop}$ provides a tighter bound than $\theta^{-\triangle}$, the strengthening of θ' by adding triangle inequalities from [9]. On the other hand for $\overline{G_{11}}$ and $\overline{G_{14}}$ we find $\nu^{(r)} < \theta^{\rm cop}$ in accordance with the theoretical results of Section 3. However, computing $\theta^{\rm cop}$ is of course much faster than $\nu^{(r)}$, which was reported to be computationally inaccessible in [17] for $\overline{G_{17}}$.

Table 1: Improvements of θ' for graphs from [17]. Here $\theta^{-\triangle}$ is the strengthening (14) from [9], and θ^{cop} results from copositivity cuts (according to the heuristic described in Section 5), whereas $\nu^{(r)}$ is the bound reported in [17] for $r = \omega - 2$.

graph	n	ω	θ'	$\theta^{-\triangle}$	θ^{cop}	$\nu^{(r)}$
$\overline{G_8}$	8	3	3.468	3.2	3	3.043
$\overline{G_{11}}$	11	4	4.694	4.386	4.28	4.011
$\overline{G_{14}}$	14	5	5.916	5.557	5.485	$\geq$5.004
$\overline{G_{17}}$	17	6	7.134	6.729	6.657	—

As a second class of special graphs we consider direct products of graphs where the θ' bound is not exact. This construction can be used to obtain graphs with even larger gaps between $\omega(\mathcal{G})$ and $\theta'(\mathcal{G})$. We build new graphs starting from the 5-cycle C_5 with $\theta'(C_5) = \sqrt{5}$ and from the Petersen graph P (of order 10) with $\theta'(P) = 2.5$ while $\omega(P) = 2$. It turns out that for $C_5 * C_5$ of order 25, we get

$$\omega = 4 < \theta^{\text{cop}} = 4.037 < \theta^{-\triangle} = 4.47 < \theta' = 5\,,$$

while for $P * C_5$ of order 50, we obtain

$$\omega = 4 < \theta^{\text{cop}} = 4.11 < \theta^{-\triangle} = 5 < \theta' = 5.59\,.$$

This effect gets even more accentuated if we restrict to the first 20, or 25 vertices of $P * C_5$, where $\theta^{\text{cop}} = 4$ is exact while all other bounds are equal to 5.

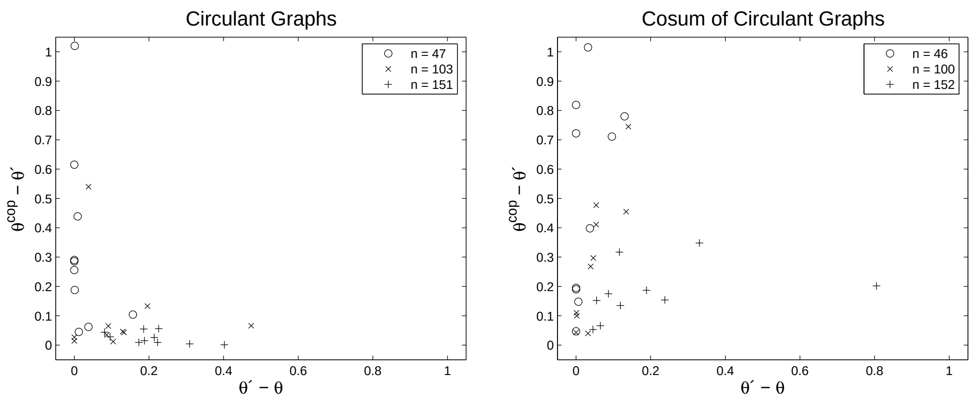
6.2 Circulant graphs and structured random tests

Circulant graphs are graphs whose adjacency matrices satisfy the following:

- $A_{i,j} = A_{1,|j-i|+1}$;
- $A_{1,j+1} = A_{1,n-j+1}$ if $1 \leq j \leq n-1$.

This class of graphs is of general interest in this context because, as proved in [3, Theorem 3.1], for some of them (in particular for those where the order

Figure 2: Improvement $\theta^{cop} - \theta'$ against $\theta' - \theta$ for randomly generated circulant graphs and cosums of circulant graphs of different orders n.



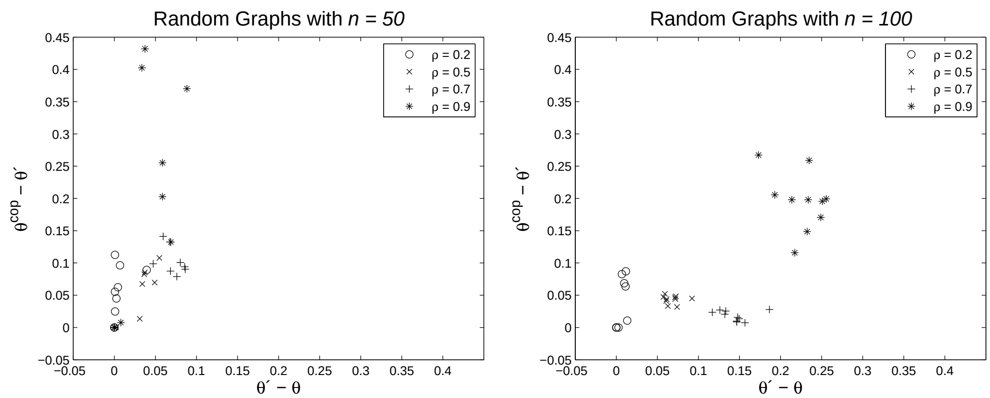
n is a prime number) it holds that $\theta'(\mathcal{G}) > \omega(\mathcal{G})$. Therefore, they form a promising class of graphs to evaluate our approach of strengthening $\theta'(\mathcal{G})$ by using copositivity cuts.

In order to test the heuristics, we generated 10 random circulant graphs of orders 47, 103 and 151, respectively, with adjacencies defined by $A_{1,j} = [0,\ 1,\ v,\ \tilde{v},\ 1]$. Here v is a random 0-1 vector (of length $m = 22$, $m = 50$ and $m = 74$ respectively), and $\tilde{v}$ the reversion of v, i.e. $\tilde{v}_i = v_{m-i}$. For all these graphs there is a gap between ω and θ' due to [3, Theorem 3.1].

In Figure 2 we plot the improvement of θ' over θ against the improvement of θ^{cop} over θ'. One can clearly see that for the smallest graphs ($n = 47$) the gain by applying cuts is quite impressive. Here in two cases θ^{cop} was smaller than the truncation of θ', thus giving an actual improvement of the bound. For $n = 103$ the gain is less impressive, but still of the same order as $\theta - \theta'$. For one instance the improvement by cuts survives truncation. Finally for $n = 151$ the gain by our cuts becomes relatively small. It is interesting to observe that $\theta - \theta'$ increases with n, whereas $\theta^{\text{cop}} - \theta'$ decreases with n. This suggests that further research is necessary to improve the heuristics of Section 5 for larger graphs.

To obtain instances of denser graphs we generated the cosum of two circulant graphs with orders n_1 and n_2, respectively, for some prime values of n_i. This choice again guarantees a gap between ω and θ'. We generated 10 random instances of order 46 (= 23+23), 100 (= 47+53) and 152 (= 73+79), respectively. To obtain improvements of θ' we ran the heuristic for a time comparable to that of computing θ'. The second part of Figure 2 shows the

Figure 3: Improvement $\theta^{\mathrm{cop}} - \theta'$ against $\theta' - \theta$ for randomly generated graphs with various densities ρ.



corresponding results.

There is again a visible trend that for larger n the improvements decrease. However, the results are much more promising than for circulant graphs before. Both for $n = 46$ and $n = 100$, the gain from the cuts is usually much larger than $\theta - \theta'$, and for $n = 152$ the improvements seem to be more or less of the same order. There were six instances with $n = 46$, three instances with $n = 100$ and two instances with $n = 152$ for which θ^{cop} was smaller than the truncation of θ'.

6.3 Unstructured random graphs

Finally we want to evaluate our heuristics on completely random graphs of various densities ρ. We generated 10 random graphs of approximate density $\rho = 0.2$, $\rho = 0.5$, $\rho = 0.7$ and $\rho = 0.9$ respectively, by choosing for each pair of nodes with probability ρ whether there is an edge or not. We considered $n = 50$ and $n = 100$.

The results presented in Figure 3 clearly illustrate the influence of ρ on the performance of our heuristics. Especially for $n = 100$ the results show clusters for different ρ. The improvement of LoMERoRuS bound over Lovász' bound $(\theta' - \theta)$ is strictly increasing with ρ. The further improvement gained by cuts $(\theta^{cop} - \theta')$ is also best for very dense graphs, but does not seem to have such a clear isotonic dependence on ρ. We observed that it was most difficult to obtain valid cuts at a density of $\rho = 0.7$. For $\rho = 0.9$ significant improvements were obtained, whereas for smaller ρ valid cuts could be found, but the gain by cutting was not that large.

For $n = 50$ there was no instance where the improvement of θ^{cop} survived truncation, but this is mainly due to the fact that for most of these instances already the Lovász' bound θ was close to ω (for 11 out of 40 instances θ was actually exact). Also for $n = 100$ and $\rho = 0.2$ Lovász' bound was in all instances very close to ω. Among the other 30 instances ($\rho \geq 0.5$) there were four for which θ^{cop} was smaller than the truncation of θ'. The results from Figure 3 again show that for $n = 50$ the gain obtained by the cuts from our heuristics is larger than for $n = 100$. We have also considered graphs with $n = 150$ and $\rho = 0.5$, and as in the case of circulant graphs the improvements become fairly small.

7 Conclusion and outlook

We conclude that the heuristics discussed here work best for graphs of comparably small order, or for highly structured graphs. It remains a topic of further research to develop heuristics which perform well for larger graphs in general. One obvious way of improvement would be simply to generate more cuts, based upon the decision how much additional computational time one is prepared to invest in generating cuts. Another improvement might be to use cuts based on graphs with a clique number larger than 3. The generation of such cuts through the greedy approach is not advisable because of the increase of the computational demand with the clique number. An idea that we would like to explore in the future is to derive valid cuts through a composition technique where a graph is obtained by taking the cosum of small subgraphs with known (and small, 2 or 3) clique number, like the subgraphs $\mathcal{H}_r$ already employed in the heuristic presented in Section 5.1: the clique number of the cosum graph would be known and equal to the sum of the subgraphs' clique numbers. It may also be fruitful to develop specific heuristics when dealing with special classes of graphs. In general one seems to find better chances for improvement in structured graphs than in unstructured ones. The instances which were presented here should demonstrate that at least in principle the use of copositivity cuts can lead to improvements of the θ' bound, even for some particularly difficult cases like the graphs introduced by Peña et al. [17].

References

[1] Bomze, I.M. (2009), "Copositive optimization," in: C.A. Floudas, P.M. Pardalos (eds.), *Encyclopedia of Optimization (2nd ed.),* pp. 561–564. Springer, New York.

[2] Bomze, I.M., M. Budinich, P. Pardalos, and M. Pelillo (1999), "The maximum clique problem," in: D.-Z. Du, P.M. Pardalos (eds.), *Handbook of Combinatorial Optimization (supp. Vol. A)*, 1–74. Kluwer, Dordrecht.

[3] Bomze, I.M., F. Frommlet, and M. Locatelli (2007), "Gap, cosum, and product properties of the θ' bound on the clique number," Technical Report TR-ISDS **2007-06**, University of Vienna, available at www.optimization-online.org/DB_FILE/2007/04/1649.pdf, last accessed 19 Feb. 2008.

[4] Bomze, I.M., M. Locatelli, and F. Tardella (2008), "New and old bounds for standard quadratic optimization: dominance, equivalence and incomparability," *Mathematical Programming* **115**, 31–64.

[5] Borchers B. (1999), "CSDP, a C library for semidefinite programming,", *Optimization Methods and Software* **11**, 613–623.

[6] Burer, S. (2008), "On the copositive representation of binary and continuous nonconvex quadratic programs," *Mathematical Programming* DOI 10.1007/s10107-008-0223-z.

[7] Busygin, S. (2009), "Copositive programming," in: C.A. Floudas, P.M. Pardalos (eds.), *Encyclopedia of Optimization (2nd ed.),* pp. 564–567. Springer, New York.

[8] de Klerk, E., and D.V. Pasechnik (2002), "Approximation of the stability number of a graph via copositive programming," *SIAM Journal of Optimization* **12**, 875–892.

[9] Dukanović, I., and F. Rendl (2007), "Semidefinite programming relaxations for graph coloring and maximal clique problems," *Mathematical Programming* **B 109**, 345–365.

[10] Gvozdenović, N., and M. Laurent, M. (2005), "Semidefinite bounds for the stability number of a graph via sums of squares of polynomials," *Lecture Notes in Computer Science*, vol 3509/2005, pages 136–151. Integer Programming and Combinatorial Optimization: 11th International IPCO Conference.

[11] Knuth, D.E. (1994), "The sandwich theorem," *Electronic Journal of Combinatorics* **22**, 1–48.

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

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

[14] Loefberg, J. (2004), "YALMIP : A Toolbox for Modeling and Optimization in MATLAB," in *Proceedings of the CACSD Conference*, Taipei, Taiwan, 2004.

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

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

[17] Peña J., J. Vera, and L. Zuluaga (2007), "Computing the stability number of a graph via linear and semidefinite programming," *SIAM Journal on Optimization* **18**, 87–105.

[18] Schrijver, A. (1979), "A comparison of the Delsarte and Lovasz bounds," *IEEE Transactions on Information Theory* **25**, 425–429.