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Research article

Gap, cosum and product properties of the θ' bound on the clique number

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In a paper published 1978, McEliece, Rodemich and Rumsey improved the θ Lovász' bound for the Maximum Clique Problem. This strengthening has become well-known under the name Lovász-Schrijver bound and is usually denoted by θ'. This article now deals with situations where this bound is not exact. To provide instances for which the gap between this bound and the actual clique number can be arbitrarily large, we establish homomorphy results for this bound under cosums and products of graphs. In particular we show that for circulant graphs of prime order there must be a positive gap between the clique number and the bound.

Keywords: Maximum clique problem; circulant graph; graph product; copositive programming; semidefinite programming

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1. Introduction

The Maximum Clique Problem (MCP) amounts to finding a complete subgraph of largest possible size in a given loopless undirected graph $\mathcal{G}$. This size is called the clique number $\omega(\mathcal{G})$. We refer to [1] for a survey about MCP. Many upper bounds have been proposed for $\omega(\mathcal{G})$. Some of these bounds are based on the solution of a semidefinite program (SDP). Among them is the famous Lovász bound [10] which is usually denoted by $\theta(\mathcal{G})$, and the strengthening $\theta'(\mathcal{G})$ of $\theta(\mathcal{G})$ which goes back to McEliece, Rodemich, and Rumsey [11], but sometimes is attributed to Schrijver [13]. This bound $\theta'(\mathcal{G})$ will be shortly reviewed in Section 2. In Section 3 we study circulant graphs and prove that for this class $\theta'(\mathcal{G}) > \omega(\mathcal{G})$ holds under certain conditions which are satisfied, e.g., if the order of $\mathcal{G}$ is prime. In Section 4 we establish homomorphy results for this bound under cosums and products of graphs in order to obtain graphs with an arbitrarily large gap between $\theta'(\mathcal{G})$ and the exact clique number $\omega(\mathcal{G})$. While the possibility of making the gap arbitrarily large is already known in the literature, cf. also [7, 8], these specific constructions give some examples where recently introduced cuts [3], added to the SDP formulation for $\theta'(\mathcal{G})$, allow for an arbitrarily large improvement over this bound.

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In the sequel, we employ the following notation: I_n is the $n \times n$ identity matrix and J_n is the all-ones $n \times n$ matrix. Let $\mathcal{S}^n$ denote the set of all symmetric $n \times n$ matrices. Then the cone of copositive $n \times n$ matrices $\mathcal{C}^n$ is defined as

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

The cone of positive-semidefinite $n \times n$ matrices is denoted by $\mathcal{P}^n \subset \mathcal{C}^n$, and the cone of symmetric $n \times n$ matrices with no negative entries by $\mathcal{N}^n \subset \mathcal{C}^n$. We will also write $A \succeq B$ to signify $A - B \in \mathcal{P}^n$, and $A \geq B$ when $A - B \in \mathcal{N}^n$ for two symmetric $n \times n$ matrices A, B. The Frobenius inner product for such matrices is denoted by $A \bullet B := \text{trace}\,(AB)$. At places we denote by $A_e = A_{kh} = A_{hk}$ an (off-diagonal) entry of a symmetric matrix A, if $e = \{k, h\}$. For such e, we denote by E_e the symmetric $n \times n$ zero-one matrix having zero entries except those at $e = \{k, h\}$, i.e., $[E_e]_e = [E_e]_{kh} = [E_e]_{hk} = 1$. Finally, the operator diag (A) extracts the diagonal of $A \in \mathcal{S}^n$, rendering a vector in n-dimensional Euclidean space $\mathbb{R}^n$. The standard simplex in this space is denoted by

$$\Delta = \{x \in \mathbb{R}^n : x_i \geq 0\,,\ \text{all} i\,,\ \sum_{i=1}^n x_i = 1\}\,.$$

2. Review of some SDP-based bounds for the clique number

Consider a loopless undirected graph $\mathcal{G} = (V_\mathcal{G}, \mathcal{E}_\mathcal{G})$ with $n \times n$ adjacency matrix $A_\mathcal{G}$ where $n = |V_\mathcal{G}|$ is the order of $\mathcal{G}$. Let $Q_\mathcal{G} = J_n - A_\mathcal{G}$. A well-known result states that the maximum clique problem (which is NP-hard) can be formulated as a copositive program [5]:

$$l(\mathcal{G}) := 1/\omega(\mathcal{G}) = \max\{\lambda : Q_\mathcal{G} - \lambda J_n \in \mathcal{C}^n\}\,. \tag{1}$$

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

$$l'(\mathcal{G}) := \max\{\lambda : Q_\mathcal{G} - \lambda J_n \in \mathcal{K}^n_0\}\,. \tag{2}$$

Obviously $l'(\mathcal{G}) \leq l(\mathcal{G})$.

The bound $\theta'(\mathcal{G})$ is an upper bound on the clique number $\omega(\mathcal{G})$ improving upon the Lovász bound [10] which is usually denoted by $\theta(\mathcal{G})$. Both bounds can be defined in various ways. One possibility is to put $\theta'(\mathcal{G}) = 1/l'(\mathcal{G})$, i.e., using (2). For (2) strong duality holds, and the dual problem is given by

$$l'(\mathcal{G}) = \min\{Q_\mathcal{G} \bullet X : J_n \bullet X = 1\,,\ X \in \mathcal{P}^n \cap \mathcal{N}^n\}\,. \tag{3}$$

From (3) we can derive the following more direct formulation:

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

where $A_{\overline{\mathcal{G}}}$ is the adjacency of the complementary graph $\overline{\mathcal{G}}$ of $\mathcal{G}$. We can also give the dual formulation of (4):

$$\theta'(\mathcal{G}) = \min\{t : tQ_\mathcal{G} - J_n \in \mathcal{K}^n_0\}\,. \tag{5}$$

The following SDP formulation of $\theta'(\mathcal{G})$ is most often used in the literature, as pointed out in [5], and at first glance seems to be stronger than (4), but is in fact equivalent:

$$\theta'(\mathcal{G}) = \max\left\{J_n \bullet X : I_n \bullet X = 1\,,\ A_{\overline{\mathcal{G}}} \bullet X = 0\,,\ X \in \mathcal{P}^n \cap \mathcal{N}^n\right\}\,. \qquad (6)$$

The dual of this formulation is

$$\theta'(\mathcal{G}) = \min\{t : tI_n + \sum_{e\in\mathcal{E}_{\overline{\mathcal{G}}}} y_e E_e + \sum_{e\in\mathcal{E}_{\mathcal{G}}} z_e E_e \succeq J_n,\ z_e \le 0\,,\ \text{all } e \in \mathcal{E}_{\mathcal{G}}\}\,. \qquad (7)$$

For later reference we recall the (dual) definition of the Lovász bound $\theta(\mathcal{G})$:

$$\theta(\mathcal{G}) = \min\{t \ : \ tI_n + \sum_{e\in\mathcal{E}_{\overline{\mathcal{G}}}} y_e E_e \succeq J_n\}\,, \qquad (8)$$

and the dual formulation of a lower bound on the chromatic number, the Szegedy bound $\theta^+(\mathcal{G})$ [14]:

$$\theta^+(\mathcal{G}) := \min\{t \ : \ tI_n + \sum_{e\in\mathcal{E}_{\overline{\mathcal{G}}}} y_e E_e \succeq J_n\,,\ y_e \ge 0\,,\ \text{all } e \in \mathcal{E}_{\overline{\mathcal{G}}}\}\,. \qquad (9)$$

From equations (7), (8), and (9), the following relation between the three bounds is immediate:

$$\omega(\mathcal{G}) \le \theta'(\mathcal{G}) \le \theta(\mathcal{G}) \le \theta^+(\mathcal{G}) \le \chi(\mathcal{G})\,.$$

Thus, for perfect graphs $\mathcal{G}$ where $\omega(\mathcal{G}) = \chi(\mathcal{G})$, all bounds above coincide. On the other hand, there are graphs with large gaps between θ and ω, e.g., $\theta(\mathcal{G})/\omega(\mathcal{G}) > n2^{-c\sqrt{\log n}}$, according to [7], and it has been shown that ω is NP-hard to approximate within a factor of $n^{1-\varepsilon}$ for an arbitrarily small $\varepsilon > 0$ [8], so in the worst case we have to expect large gaps also between θ' and ω. However, construction of concrete instances is not obvious by these theoretical results, and this is the purpose for the subsequent sections.

3. Circulant graphs

A matrix A is a *circulant* matrix, if it satisfies the Toeplitz condition $A_{i,j} = A_{1,|j-i|+1}$ and in addition $A_{i,j+1} = A_{1,n-j+1}$ for $1 \le j \le n-1$. A graph $\mathcal{G}$ is called *circulant*, if its adjacency matrix $A = A_{\mathcal{G}}$ is a circulant matrix. This class of graphs is of general interest in this context, because, as we prove in the following theorem, for most of them $\theta'(\mathcal{G}) > \omega(\mathcal{G})$. The proof follows the ideas used for odd cycles in [12].

Theorem 3.1 : *If G is a circulant graph of size n with the clique number $\omega \ge 2$, and if there exists a maximum clique $S \subseteq V_{\mathcal{G}}$ such that $\sum_{j\in S} \xi^j \ne 0$ for any n-th unitary root ξ, then $\theta'(\mathcal{G}) > \omega$.*

Proof: Assume that $\theta'(\mathcal{G}) = \omega$, and denote $Q := Q_{\mathcal{G}}$. Then by (2) we have $Q - \frac{1}{\omega}J_n \in \mathcal{K}_0^n = \mathcal{P} + \mathcal{N}$. Since $P \in \mathcal{P}$ implies $P = \sqrt{P}\sqrt{P}$,

$$Q - \frac{1}{\omega}J_n = RR + N, \qquad R \in \mathcal{S}^n, N \in \mathcal{N}^n.$$

If we could show that $R = 0$, then $Q - \frac{1}{\omega} J_n = N \geq 0$ which is a contradiction as $Q_{ij} = 0$ for any edge $ij \in \mathcal{E}_{\mathcal{G}}$. To this aim let r_j denote the j-th column of R. For any maximum clique $S \subseteq V_{\mathcal{G}}$ of size ω we have $Q_{i,j} = 0$, if $i \neq j$ and $\{i, j\} \subseteq S$. Let χ_S be the characteristic vector of S. So $\chi_S^T Q \chi_S = \omega$, and $\chi_S(Q - \frac{1}{\omega} J_n)\chi_S = 0$. On the other hand by computing the same quadratic form $\chi_S^T(RR + N)\chi_S$ we obtain

$$0 = ||\sum_{j \in S} r_j||^2 + \sum_{i,j \in S} N_{i,j} \geq ||\sum_{j \in S} r_j||^2,$$

and we conclude that $\sum_{j \in S} r_j = 0$. In what follows summation over indices is always to be taken modulo n. Let $S = j_1, ..., j_\omega$ be a maximum clique. Due to the definition of circulant graphs $S_{k+1} = j_1 + k, ..., j_n + k$ is also a maximum clique, and therefore with the same arguments we get $\sum_{j \in S} r_{j+k} = 0$. Next we define M as the $n \times n$ matrix where the k-th row is given by the characteristic vector of S_k. By definition $\chi_{S_k} R^T = \sum_{j \in S} r_{j+k} = 0$ is just the k-th row of the product MR^T. So $MR^T = 0$. Now obviously, if M has full rank (is invertible), then $R^T = 0$. But M is a circulant matrix for which it is well known that the eigenvalues can be calculated by using discrete Fourier transform. Specifically, the condition for an eigenvalue 0 is that there exists k such that $\sum_{j=1}^{n} M_{1,j}\ e^{\frac{2\pi k}{n}} = 0$ which we do not allow for by assumption. □

The problem under which conditions the sum of unitary roots becomes 0 has been well studied in the literature (see, e.g., [4]). For our purposes it is sufficient to remark that, if n is a prime number, then there is no solution to $\sum_{0 \leq j_1 < \cdots < j_\omega < n} \xi^{j_l} = 0$ where ξ is an n-th unitary root. So when n is a prime number, for all $1 < \omega < n$ we have $\theta'(\mathcal{G}) > \omega = \omega(\mathcal{G})$. This makes the class of circulant graphs ideal to evaluate procedures for improving the θ' bound. The following section exhibits constructions where any positive gap can be blown up to an arbitrary size. After all, the improvement should also survive truncation as of course also $\lfloor \theta' \rfloor$ is a valid upper bound for the clique number.

4. Sums and products of graphs

In this section we want to construct graphs with large gaps between the clique number and the θ' bound by using cosums and various products. The idea has been inspired by Knuth [9] who proved that the Lovász number is an additive homomorphism for the cosum and a multiplicative homomorphism for the direct product and the direct coproduct. To the best of our knowledge analogous results for the θ' bound have not yet been established.

4.1. *Cosums*

The (direct) sum of two graphs $\mathcal{G}_1 = (V_{\mathcal{G}_1}, \mathcal{E}_{\mathcal{G}_1})$ and $\mathcal{G}_2 = (V_{\mathcal{G}_2}, \mathcal{E}_{\mathcal{G}_2})$ with disjoint vertex sets $V_{\mathcal{G}_i}$ of size n_i is simply the graph $\mathcal{G} = (V_{\mathcal{G}_1} \cup V_{\mathcal{G}_2}, \mathcal{E}_{\mathcal{G}_1} \cup \mathcal{E}_{\mathcal{G}_2})$. This means no edges are added to the disjoint union, in terms of adjacencies

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

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 $V_{\mathcal{G}_1} \cup V_{\mathcal{G}_2}$, but now $\{u, v\}$ 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. Obviously, a vertex subset C with $C_i = C \cap V_{\mathcal{G}_i}$ is a clique in $\mathcal{G}_1 \oplus \mathcal{G}_2$, if and only if C_i is a clique in $\mathcal{G}_i$ for $i = 1, 2$ so that $\omega(\mathcal{G}_1 \oplus \mathcal{G}_2) = \omega(\mathcal{G}_1) + \omega(\mathcal{G}_2)$. We will show that the same holds for θ'.

Theorem 4.1: *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be graphs with disjoint vertex sets, then*

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

Proof: First we note that the claimed equality is equivalent to

$$l'(\mathcal{G}_1 \oplus \mathcal{G}_2) = \frac{l'(\mathcal{G}_1) l'(\mathcal{G}_2)}{l'(\mathcal{G}_1) + l'(\mathcal{G}_2)}.$$

In [2] it was proved that bound (2) is equivalent to the best convex/vertex-optimal decomposition (`cvd`) bound. A `cvd` decomposes a nonnegative symmetric square matrix Q as follows:

$$Q = P + N, \quad P \in \mathcal{P}^n, \quad N \in \mathcal{N}^n \;\text{ with diag } (N) = 0\,.$$

The above decomposition gives a lower bound $\min_{x \in \Delta} x^\top P x$ for the Standard Quadratic optimization problem $\min_{x \in \Delta} x^\top Q x$ where Δ is the standard simplex in $\mathbb{R}^n$. The best possible `cvd` is one for which this lower bound is as high as possible.

Now, let us compute the best `cvd` bound for the cosum graph $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$ of order $n = n_1 + n_2$. We have, abbreviating $Q_i = Q_{\mathcal{G}_i}$, that

$$Q_{\mathcal{G}} = I_n + A_{\overline{\mathcal{G}_1 \oplus \mathcal{G}_2}} = \begin{bmatrix} I_{n_1} + A_{\overline{\mathcal{G}}_1} & O \\ O & I_{n_2} + A_{\overline{\mathcal{G}}_2} \end{bmatrix} = \begin{bmatrix} Q_1 & O \\ O & Q_2 \end{bmatrix}.$$

The `cvd`s for such a Q matrix are as follows

$$\begin{bmatrix} P_1 & -Z \\ -Z & P_2 \end{bmatrix} + \begin{bmatrix} N_1 & Z \\ Z & N_2 \end{bmatrix}$$

where we must have that $Z \geq O$, and necessarily $P_i + N_i$ are `cvd` for Q_i. First we note that the best bound is certainly obtained when $Z = O$. Indeed,

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

and the bound given by the latter matrix is at least as good as the one given by the former. Componentwise any $x \in \Delta$ can be seen as $x = [\lambda x_1, (1-\lambda) x_2]$ with $x_i \in \Delta_i$ where $\Delta_i \subset \mathbb{R} n_i$ are again standard simplices. This implies that the bound given by the latter matrix is obtained by solving the following simple one-dimensional problem

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

with $\pi_i = \min_{x \in \Delta} x^\top P_i x > 0$. Thus the best possible such bound is obtained if

$P_i + N_i$ are optimal cvds for Q_i, i.e., if

$$\pi_i = \min_{x \in \Delta} x^\top P_i x = l'(\mathcal{G}_i) \quad \text{for } i = 1, 2\,,$$

wherefrom the result on the cosum follows. $\square$

Note that, according to Theorems 3.1 and 4.1, we can build graphs with an arbitrarily large gap between the θ' bound and the clique number by taking the cosum of a sufficiently large number of circulant graphs of prime order.

4.2. *Products*

For products of the two graphs $\mathcal{G}_1$ and $\mathcal{G}_2$ we consider the vertex set of $n = n_1 n_2$ ordered pairs $V_{\mathcal{G}_1} \times V_{\mathcal{G}_2}$. We will define several different products in terms of adjacencies using the Kronecker product $\otimes$ which transforms any two symmetric binary matrices of order n_i $(i = 1, 2)$ into a symmetric binary $n \times n$ matrix. Again we write $Q_i := J_{n_i} - A_{\mathcal{G}_i}$.

The *direct* or *strong product* $\mathcal{G}_1 * \mathcal{G}_2$ is defined via

$$A_{\mathcal{G}_1 * \mathcal{G}_2} := I_{n_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes I_{n_2} + A_{\mathcal{G}_1} \otimes A_{\mathcal{G}_2} \tag{10}$$

or equivalently $I_n + A_{\mathcal{G}_1 * \mathcal{G}_2} = (I_{n_1} + A_{\mathcal{G}_1}) \otimes (I_{n_2} + A_{\mathcal{G}_2})$ which is the same as

$$Q_{\overline{\mathcal{G}_1 * \mathcal{G}_2}} = Q_{\overline{\mathcal{G}}_1} \otimes Q_{\overline{\mathcal{G}}_2}\,. \tag{11}$$

The *direct coproduct* is $\mathcal{G}_1 \,\overline{*}\, \mathcal{G}_2 = \overline{\overline{\mathcal{G}}_1 * \overline{\mathcal{G}}_2}$. Complementation of (11) gives $Q_{\mathcal{G}_1 \overline{*} \mathcal{G}_2} = Q_1 \otimes Q_2$ or after some manipulations,

$$A_{\mathcal{G}_1 \overline{*} \mathcal{G}_2} = Q_1 \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes J_{n_2}\,. \tag{12}$$

The *lexicographical product* $\mathcal{G}_1 \,\tilde{*}\, \mathcal{G}_2$ is defined via

$$A_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2} := I_{n_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes J_{n_2}\,. \tag{13}$$

One may also consider another lexicographical product $J_{n_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes I_{n_2}$, leading to graphs with similar properties.

From (10), (12) and (13) it is immediately clear that

$$A_{\mathcal{G}_1 * \mathcal{G}_2} \le A_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2} \le A_{\mathcal{G}_1 \overline{*} \mathcal{G}_2}\,. \tag{14}$$

Knuth [9] has proven for the Lovász number that $\theta(\mathcal{G}_1 * \mathcal{G}_2) = \theta(\mathcal{G}_1 \overline{*} \mathcal{G}_2) = \theta(\mathcal{G}_1)\theta(\mathcal{G}_2)$. For each of the three graph products introduced above it is easy to prove that the θ' bound of the product graph is at least as large as the product of the θ' bounds of its factors. This is stated in the following observation.

Observation 4.2 If $\mathcal{G}_1$ and $\mathcal{G}_2$ are graphs with disjoint vertex sets, then

$$\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) \le \theta'(\mathcal{G}_1 * \mathcal{G}_2) \le \theta'(\mathcal{G}_1 \tilde{*} \mathcal{G}_2) \le \theta'(\mathcal{G}_1 \overline{*} \mathcal{G}_2)\,. \tag{15}$$

Proof: If $O \leq A \leq B$ and $\mathcal{M} \subseteq \mathcal{N}$, then

$$\{X \in \mathcal{M} : B \bullet X = 0\} \subseteq \{X \in \mathcal{M} : A \bullet X = 0\} \,.$$

Since complementation reverses the order in (14) it follows now from (6) that $\theta'(\mathcal{G}_1 * \mathcal{G}_2) \leq \theta'(\mathcal{G}_1 \tilde{*} \mathcal{G}_2) \leq \theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_2)$. Thus it suffices to prove that $\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) \leq \theta'(\mathcal{G}_1 * \mathcal{G}_2)$. To this end we define $\theta_p := \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2)$. Let $X_1^\star$ and $X_2^\star$ be optimal solutions of $\theta'(\mathcal{G}_1)$ and $\theta'(\mathcal{G}_2)$ respectively, according to formulation (6). Noting that the Kronecker product of positive-semidefinite matrices is again positive-semidefinite it is easy to see that $X^\otimes := X_1^\star \otimes X_2^\star$ is (6)-feasible for $\theta'(\mathcal{G}_1 * \mathcal{G}_2)$. By exploiting well known properties of the Kronecker product we have that

$$\begin{aligned} J_n \bullet X^\otimes &= \text{trace }(J_{n_1} \otimes J_{n_2})(X_1^\star \otimes X_2^\star) = \text{trace }((J_{n_1}X_1^\star) \otimes (J_{n_2}X_2^\star)) \\ &= \text{trace }(J_{n_1}X_1^\star)\text{trace }(J_{n_2}X_2^\star) = \theta_p \,, \end{aligned}$$

from which the inequality follows. □

The following theorem specifies various conditions under which the inequalities in (15) can be turned into equalities.

Theorem 4.3: *Let $\mathcal{G}_1 = (V_{\mathcal{G}_1}, \mathcal{E}_{\mathcal{G}_1})$ and $\mathcal{G}_2 = (V_{\mathcal{G}_2}, \mathcal{E}_{\mathcal{G}_2})$ be two graphs with disjoint vertex sets, and let $\mathcal{G}_1 \circ \mathcal{G}_2$ be the product graph, where $\circ \in \{*, \tilde{*}, \bar{*}\}$. In the following cases:*

- **a)** $\theta(\mathcal{G}_i) = \theta'(\mathcal{G}_i)$ *for both* $i = 1, 2$, *and* $\circ \in \{\tilde{*}, \bar{*}\}$,
- **b)** $\theta(\mathcal{G}_i) = \theta'(\mathcal{G}_i)$ *for* $i = 1$ *or* $i = 2$, *and* $\circ = *$,
- **c)** $\theta^+(\mathcal{G}_i) = \theta'(\mathcal{G}_i)$ *for* $i = 1$ *or* $i = 2$, *and* $\circ = \bar{*}$,
- **d)** $[\theta(\mathcal{G}_1) - \theta'(\mathcal{G}_1)]\,[\theta^+(\mathcal{G}_2) - \theta'(\mathcal{G}_2)] = 0$ *and* $\circ = \tilde{*}$,

it holds that

$$\theta'(\mathcal{G}_1 \circ \mathcal{G}_2) = \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) \,.$$

Proof: **a)** This is the simplest case. Indeed, it obviously holds that

$$\theta'(\mathcal{G}_1 \circ \mathcal{G}_2) \leq \theta(\mathcal{G}_1 \circ \mathcal{G}_2) = \theta(\mathcal{G}_1)\theta(\mathcal{G}_2)$$

where the equality follows from the already mentioned properties of the Lovász bound. Then under the given assumption

$$\theta'(\mathcal{G}_1 \circ \mathcal{G}_2) \leq \theta(\mathcal{G}_1)\theta(\mathcal{G}_2) = \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2)$$

which, together with Observation 4.2, proves equality. Note that the result obviously holds also for $\circ = *$, but we will now see that for this case the milder requirement b) is enough.
b) Let $X_i^\star$ be the optimal solution of (6) for graph $\mathcal{G}_i$, $i = 1, 2$, and let

$$M^{i\star} := t^{i\star} I_{n_i} + \sum_{e \in \mathcal{E}_{\overline{\mathcal{G}_i}}} y_e^{i\star} E_e + \sum_{e \in \mathcal{E}_{\mathcal{G}_i}} z_e^{i\star} E_e \,,$$

with $z_e^{i\star} \leq 0$ for all $e \in \mathcal{E}_{\mathcal{G}_i}$, be the optimal solution of the dual problem (7). As already remarked in Observation 4.2, $X^\otimes = X_1^\star \otimes X_2^\star$ is a feasible solution of (6) for graph $\mathcal{G}_1 * \mathcal{G}_2$ with objective function value equal to $\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2)$, while $M^\otimes = M^{1\star} \otimes M^{2\star}$ is a complementary solution to $X^\otimes$, possibly dually infeasible.

However, we will prove feasibility of $M^{\otimes}$ w.r.t. (7). This establishes optimality of $X^{\otimes}$ and $M^{\otimes}$ for the primal and the dual, respectively. Consequently, we then arrive at

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

In order to prove dual feasibility for $M^{\otimes}$, we first need to show that $M^{\otimes} \succeq J_n$. By dual feasibility of $M^{i\star}$, $i = 1, 2$, we know that

$$M^{i\star} \succeq J_{n_i} \succeq O, \qquad i = 1, 2\,.$$

Since the Kronecker product of two positive-semidefinite matrices is still positive-semidefinite,

$$(M^{1\star} - J_{n_1}) \otimes J_{n_2} \succeq O \quad \text{and} \quad M^{1\star} \otimes (M^{2\star} - J_{n_2}) \succeq O.$$

Therefore

$$M^{1\star} \otimes M^{2\star} \succeq M^{1\star} \otimes J_{n_2} \succeq J_{n_1} \otimes J_{n_2} = J_n.$$

Next we need to prove that all the entries of $M^{\otimes}$ corresponding to edges of $\mathcal{G}_1 * \mathcal{G}_2$ are nonpositive. In order to do that, we split each graph $\mathcal{G}_i$, $i = 1, 2$, into two subgraphs $\mathcal{G}_i^{=}$ and $\mathcal{G}_i^{<}$ with edge sets defined as follows:

$$\mathcal{E}_{\mathcal{G}_i^{=}} := \{e \in \mathcal{E}_{\mathcal{G}_i} \;:\; z_e^{i\star} = 0\} \quad \text{and} \quad \mathcal{E}_{\mathcal{G}_i^{<}} := \{e \in \mathcal{E}_{\mathcal{G}_i} \;:\; z_e^{i\star} < 0\}\,.$$

Then, we have that $A_{\mathcal{G}_i} = A_{\mathcal{G}_i^{=}} + A_{\mathcal{G}_i^{<}}$ and consequently

$$\begin{aligned} A_{\mathcal{G}_1 * \mathcal{G}_2} &= I_{n_1} \otimes (A_{\mathcal{G}_2^{=}} + A_{\mathcal{G}_2^{<}}) + (A_{\mathcal{G}_1^{=}} + A_{\mathcal{G}_1^{<}}) \otimes I_{n_2} + (A_{\mathcal{G}_1^{=}} + A_{\mathcal{G}_1^{<}}) \otimes (A_{\mathcal{G}_2^{=}} + A_{\mathcal{G}_2^{<}}) \\ &= I_{n_1} \otimes A_{\mathcal{G}_2^{=}} + I_{n_1} \otimes A_{\mathcal{G}_2^{<}} + A_{\mathcal{G}_1^{=}} \otimes I_{n_2} + A_{\mathcal{G}_1^{<}} \otimes I_{n_2} + A_{\mathcal{G}_1^{=}} \otimes A_{\mathcal{G}_2^{=}} + \\ &\quad + A_{\mathcal{G}_1^{=}} \otimes A_{\mathcal{G}_2^{<}} + A_{\mathcal{G}_1^{<}} \otimes A_{\mathcal{G}_2^{=}} + A_{\mathcal{G}_1^{<}} \otimes A_{\mathcal{G}_2^{<}}\,. \end{aligned}$$

In view of the definitions of $\mathcal{G}_i^{=}$ and $\mathcal{G}_i^{<}$, we notice that the only entries in $M^{\otimes}$ corresponding to edges of $\mathcal{G}_1 * \mathcal{G}_2$ which can be strictly positive (thus violating dual feasibility) are those in $A_{\mathcal{G}_1^{<}} \otimes A_{\mathcal{G}_2^{<}}$. Then, if either $\mathcal{G}_1^{<}$ or $\mathcal{G}_2^{<}$ are empty graphs, we have dual feasibility. But if, e.g., $\theta'(\mathcal{G}_1) = \theta(\mathcal{G}_1)$, then there exists a solution $M^{1\star}$ which is optimal both for (7) and for (8) and such that $z_e^{1\star} = 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1}$, i.e., $\mathcal{G}_1^{<}$ is empty, as we wanted to prove.

c) As in part b) we are now only imposing a condition on one of the two graphs, but this condition is stronger than in b) since it asks for equality between the Szegedy and the θ' bound in one of the two factor graphs. We remark that such equality certainly holds, if a factor graph is perfect. The proof will follow an approach similar to the one employed in part b), wherefrom we take the definitions of $X^{\otimes}$ and $M^{\otimes}$. So let us assume that $\theta^{+}(\mathcal{G}_1) = \theta'(\mathcal{G}_1)$; the proof is analoguous if equality holds for $\mathcal{G}_2$. Now if $\theta^{+}(\mathcal{G}_1) = \theta'(\mathcal{G}_1)$ then an optimal solution for (9) exists which is also optimal for (7). Basically, we have the following matrix solution for $\mathcal{G}_1$:

$$M^{1\star} = t^{1\star} I_{n_1} + \sum_{e \in \mathcal{E}_{\overline{\mathcal{G}_1}}} y_e^{1\star} E_e$$

with $y_e^{1\star} \geq 0$ for all $e \in \mathcal{E}_{\overline{\mathcal{G}}_1}$. What we would like to prove is that $M^{\otimes}$ is a feasible solution of the dual (7) for the graph $\mathcal{G}_1 \bar{*} \mathcal{G}_2$ (if this holds for $\mathcal{G}_1 \bar{*} \mathcal{G}_2$, it certainly holds also for $\mathcal{G}_1 \tilde{*} \mathcal{G}_2$). Since $M^\otimes \succeq J_n$ has been already proved in part b), we only need to prove that $M_e^\otimes \le 0$ for each $e \in \mathcal{E}_{G_1 \bar{*} G_2}$. The adjacency matrix of $\mathcal{G}_1 \bar{*} \mathcal{G}_2$ is

$$(J_{n_1} - A_{\mathcal{G}_1}) \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes J_{n_2} \, .$$

Since $z_e^{1\star} = 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1}$, the entries in $A_{\mathcal{G}_1} \otimes J_{n_2}$ are all equal to zero, while since $t^{1\star} \ge 0$ and $y_e^{1\star} \ge 0$ for all $e \in \mathcal{E}_{\overline{\mathcal{G}_1}}$ and $z_e^{2\star} \le 0$ for all $e \in \mathcal{E}_{\mathcal{G}_2}$, it also holds that no entries in $(J_{n_1} - A_{\mathcal{G}_1}) \otimes A_{\mathcal{G}_2}$ are positive.

d) It is interesting to note that this is an asymmetric condition with respect to $\mathcal{G}_1$ and $\mathcal{G}_2$, asking for the same condition as in b) for $\mathcal{G}_1$ and for the same condition as in c) for $\mathcal{G}_2$. $X^\otimes$ and $M^\otimes$ are defined as above, and we still want to prove that $M^\otimes$ is a feasible solution of the dual (7) for the graph $\mathcal{G}_1 \tilde{*} \mathcal{G}_2$. Note that $M^\otimes \succeq J_n$ has been already proved in part b). First we assume that $\theta'(\mathcal{G}_1) = \theta(\mathcal{G}_1)$. Under such assumption we have that there exists an optimal solution for (8) which is also optimal for (7), i.e., we have the following matrix solution for $\mathcal{G}_1$:

$$M^{1\star} = t^{1\star} I_{n_1} + \sum_{e \in \mathcal{E}_{\overline{\mathcal{G}}_1}} y_e^{1\star} E_e \, .$$

We only need to prove that $M_e^\otimes \le 0$ for each $e \in \mathcal{E}_{G_1 \tilde{*} G_2}$. The adjacency matrix of $\mathcal{G}_1 \tilde{*} \mathcal{G}_2$ is

$$I_{n_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes J_{n_2} \, .$$

Since $t^{1\star} \ge 0$ and $z_e^{2\star} \le 0$ for all $e \in \mathcal{E}_{\mathcal{G}_2}$, as well as $z_e^{1\star} = 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1}$, it immediately follows that $M_e^\otimes \le 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2}$.

Next we assume that $\theta'(\mathcal{G}_2) = \theta^+(\mathcal{G}_2)$. Under such assumption we have that there exists an optimal solution for (9) which is also optimal for (7), i.e., we have the following matrix solution for $\mathcal{G}_2$:

$$M^{2\star} = t^{2\star} I_{n_2} + \sum_{e \in \mathcal{E}_{\overline{\mathcal{G}}_2}} y_e^{2\star} E_e \ge O \, ,$$

because $y_e^{2\star} \ge 0$ for all $e \in \mathcal{E}_{\overline{\mathcal{G}}_2}$ and $t^{2\star} \ge 0$. Since $z_e^{1\star} \le 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1}$ and $z_e^{2\star} = 0$ for all $e \in \mathcal{E}_{\mathcal{G}_2}$, it follows that $M_e^\otimes \le 0$ for all $e \in \mathcal{E}_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2}$. □

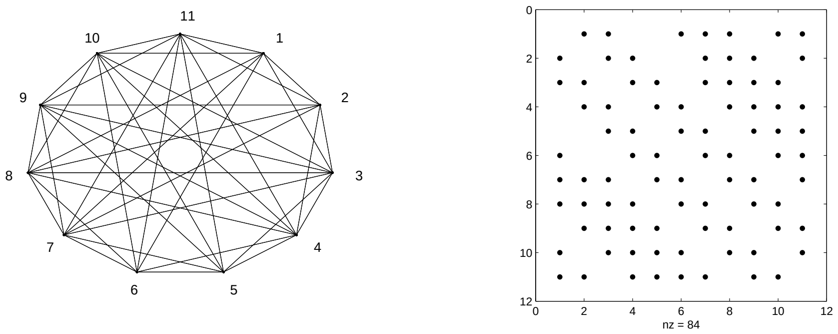
As for cosums, the above results allow to build graphs for which the gap between the θ' bound and the clique number is arbitrarily large. As an example we will look at the special case where $\mathcal{G}_1 = K_n$, the complete graph of size n, and $\mathcal{G}_2 = C_5$, the 5-cycle.

Example 4.4 It is well known that the 5-cycle 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 $\mathcal{G}_n := K_n * C_5$. In view of Theorem 4.3 we have 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.

We remark that the possibility of making the gap arbitrarily large is well-known in the community, but instances like the one above allow to show superiority of bounds which satisfy multiplicativity like the θ' bound, but rather are exact on the factors, so that an arbitrarily large improvement of the θ' bound is established, see [3].

Figure 1. A small graph $\mathcal{G}_1$ for which $[\theta'(\mathcal{G}_1)]^2 < \theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_1)$.

a) Graph b) Adjacency



The proof of Theorem 4.3 also suggests that equality between the θ' bound of the graph product and the product of the θ' bounds of its factors does *not* always hold. Indeed, $X^{\otimes}$ and $M^{\otimes}$ as defined in the proof of the theorem are complementary primal and dual solutions with $X^{\otimes}$ always primally feasible, as proved in Observation 4.2, while $M^{\otimes}$ is dually *infeasible*, if the conditions of Theorem 4.3 are not fulfilled. This suggests that the value of the primally feasible solution $X^{\otimes}$ which is equal to the product of the θ' bounds of the two factors might be improved thus leading to strict inequality between the θ' bound of the graph product and the product of the θ' bounds of its factors. Therefore, we searched for a graph for which strict inequality holds between the Lovász and the θ' bound, and considered the product of this graph with itself so that none of the conditions of Theorem 4.3 holds.

Example 4.5 The smallest circulant graph for which $\omega < \theta' < \theta$ has 16 nodes, but we individuated a smaller graph $\mathcal{G}_1$ with only 11 nodes having this property by removing the two edges $\{1, 5\}$ and $\{2, 6\}$ from a circulant graph (compare Figure 1). It holds that $\theta(\mathcal{G}_1) = 5.265 > 5.239 = \theta'(\mathcal{G}_1)$ while

$$\theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_1) = 27.486 > 27.449 = [\theta'(\mathcal{G}_1)]^2$$

thus giving an example for which strict inequality holds in Observation 4.2.

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