

Exactness of Parrilo’s conic approximations for copositive matrices and associated low order bounds for the stability number of a graph

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Abstract

De Klerk and Pasechnik (2002) introduced the bounds $\vartheta^{(r)}(G)$ ($r \in \mathbb{N}$) for the stability number $\alpha(G)$ of a graph G and conjectured exactness at order $\alpha(G) - 1$: $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$. These bounds rely on the conic approximations $\mathcal{K}_n^{(r)}$ by Parrilo (2000) for the copositive cone COP_n . A difficulty in the convergence analysis of $\vartheta^{(r)}$ is the bad behaviour of the cones $\mathcal{K}_n^{(r)}$ under adding a zero row/column: when applied to a matrix not in $\mathcal{K}_n^{(0)}$ this gives a matrix not in any $\mathcal{K}_{n+1}^{(r)}$, thereby showing strict inclusion $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subset \text{COP}_n$ for $n \geq 6$. We investigate the graphs with $\vartheta^{(r)}(G) = \alpha(G)$ for $r = 0, 1$: we algorithmically reduce testing exactness of $\vartheta^{(0)}$ to acritical graphs, we characterize critical graphs with $\vartheta^{(0)}$ exact, and we exhibit graphs for which exactness of $\vartheta^{(1)}$ is not preserved under adding an isolated node. This disproves a conjecture by Gvozdenović and Laurent (2007) which, if true, would have implied the above conjecture by de Klerk and Pasechnik.

Keywords stable set problem · α -critical graph · sum-of-squares polynomial · copositive matrix · semidefinite programming · Shor relaxation

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1 Introduction

The problem of computing the *stability number* $\alpha(G)$ of a graph $G = (V = [n], E)$, defined as the maximum cardinality of a stable set in G , is a central problem in combinatorial optimization with a wide range of applications (e.g., to scheduling, social networks analysis, genetics and chemistry, see [1], [33], [15] and references therein). This problem is well-known to be NP-hard [16], which motivates the study of tractable approximations obtained by means of linear or semidefinite relaxations. In this paper we investigate some semidefinite bounds $\vartheta^{(r)}(G)$ ($r \in \mathbb{N}$) that were introduced in [5], with a special focus on the question of understanding for which graphs the bounds are exact, especially for low order $r = 0$ and $r = 1$. Exactness of the bounds is closely related to the question whether certain associated graph matrices M_G admit copositivity certificates of semidefinite type or, equivalently, whether certain associated graph polynomials F_G admit nonnegativity certificates in terms of sums of squares.

The starting point to define these notions is the following copositive reformulation from [5] for the stability number:

$$\alpha(G) = \min\{t : t(I + A_G) - J \in \text{COP}_n\}. \quad (1.1)$$

Here, A_G , I and J denote, respectively, the adjacency matrix of G , the identity matrix and the all-ones matrix, and COP_n is the cone of copositive matrices defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \geq 0 \text{ for all } x \in \mathbb{R}^n\},$$

setting $x^{\circ 2} = (x_1^2, \dots, x_n^2)$. Since the minimum is attained in program (1.1) the following *graph matrix*

$$M_G := \alpha(G)(A_G + I) - J \quad (1.2)$$

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is copositive or, equivalently, the following *graph polynomial*

$$F_G(x) := (x^{\circ 2})^T M_G x^{\circ 2} \quad (1.3)$$

is nonnegative on \mathbb{R}^n . A natural question is whether there exist certificates for copositivity of M_G based on semidefinite programming and whether there exist certificates of nonnegativity for F_G based on sums of squares of polynomials. Such certificates can be designed using the hierarchy of inner approximations for the copositive cone COP_n proposed by Parrilo [24], and defined by

$$\mathcal{K}_n^{(r)} = \{M \in \mathcal{S}^n : (\sum_{i=1}^n x_i^2)^r (x^{\circ 2})^T M x^{\circ 2} \in \Sigma\} \quad \text{for } r \in \mathbb{N}, \quad (1.4)$$

where Σ denotes the cone of sums of squares of polynomials. These cones satisfy $\mathcal{K}_n^{(r)} \subseteq \mathcal{K}_n^{(r+1)} \subseteq \text{COP}_n$ and they cover the interior of the copositive cone:

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n. \quad (1.5)$$

Starting from the copositive formulation (1.1) and using the cones $\mathcal{K}_n^{(r)}$, de Klerk and Pasechnik [5] introduced the following hierarchy of approximations for $\alpha(G)$:

$$\vartheta^{(r)}(G) = \min\{t : t(A_G + I) - J \in \mathcal{K}_n^{(r)}\}, \quad (1.6)$$

which satisfy $\alpha(G) \leq \vartheta^{(r+1)}(G) \leq \vartheta^{(r)}(G)$ for all $r \in \mathbb{N}$ and $\lim_{r \rightarrow \infty} \vartheta^{(r)}(G) = \alpha(G)$. Note the minimum is indeed attained in program (1.6). As sums of squares of polynomials can be modelled using semidefinite programming each bound $\vartheta^{(r)}(G)$ is defined via a semidefinite program. The bound is said to be *exact at order* r if $\vartheta^{(r)}(G) = \alpha(G)$.

Yet another useful notion is the parameter ϑ -rank(G), called the ϑ -rank of G , which is defined in [19] as the smallest integer r for which $\vartheta^{(r)}(G) = \alpha(G)$, setting ϑ -rank(G) = ∞ if no such r exists.

For clarity let us summarize the following links between the above notions: for any integer $r \in \mathbb{N}$ we have

$$M_G \in \mathcal{K}_n^{(r)} \iff (\sum_{i=1}^n x_i^2)^r F_G \in \Sigma \iff \vartheta^{(r)}(G) = \alpha(G) \iff \vartheta\text{-rank}(G) \leq r. \quad (1.7)$$

De Klerk and Pasechnik [5] conjectured that the hierarchy $\vartheta^{(r)}(G)$ converges to $\alpha(G)$ in at most $\alpha(G) - 1$ steps, which would show that this continuous copositive-based hierarchy has the same convergence behaviour as the Lasserre hierarchy based on discrete formulations of $\alpha(G)$ [17, 18]. In view of (1.7) this can be reformulated as follows.

Conjecture 1.1 ([5]). *For a graph G , any of the following equivalent claims holds: (i) $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$, (ii) $(\sum_{i=1}^n x_i^2)^{\alpha(G)-1} F_G \in \Sigma$, (iii) $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$, (iv) ϑ -rank(G) $\leq \alpha(G) - 1$.*

The weaker conjecture asking whether finite convergence holds at *some* order $r \in \mathbb{N}$ is also open.

Conjecture 1.2 ([19]). *For a graph G , any of the following equivalent claims holds: (i) $M_G \in \bigcup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)}$, (ii) $(\sum_{i=1}^n x_i^2)^r F_G \in \Sigma$ for some $r \in \mathbb{N}$, (iii) $\vartheta^{(r)}(G) = \alpha(G)$ for some $r \in \mathbb{N}$, (iv) ϑ -rank(G) $< \infty$.*

Let us recap some of the main known results about these conjectures. In [12] Conjecture 1 was shown to hold for all graphs with $\alpha(G) \leq 8$ (see also [31] for the case $\alpha(G) \leq 6$). In [19] it was observed that it suffices to prove both Conjectures 1 and 2 for the class of critical graphs, i.e., for the graphs G satisfying $\alpha(G \setminus e) = \alpha(G) + 1$ for all edges e of G . In addition, it is shown in [19] that Conjecture 2 holds for acritical graphs, i.e., for the graphs G satisfying $\alpha(G \setminus e) = \alpha(G)$ for all edges.

Some possible directions for resolving Conjectures 1.1 and 1.2. In what follows we mention some possible strategies that could be followed to attack the above two conjectures along with their pitfalls.

A first idea is to investigate whether one can exploit the fact that any graph matrix M_G has its diagonal entries that all take the same value (equal to $\alpha(G) - 1$). Indeed it is conjectured in [7] that any copositive matrix with diagonal entries 0 or 1 belongs to some cone $\mathcal{K}_n^{(r)}$ and it is shown that this is true for matrix size $n = 5$ (with $r = 1$ in that case). Hence a positive answer to this conjecture would immediately imply that M_G belongs to some cone $\mathcal{K}_n^{(r)}$ and thus settle Conjecture 1.2. However, we will disprove the above conjecture from [7] for matrix size $n \geq 6$ (see Section 3). In particular, this shows that the inclusion $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$ in (1.5) is strict for any $n \geq 6$.

A second possible strategy is to consider the impact of adding an isolated node. Let $G \oplus i_0$ denote the graph obtained by adding i_0 as an isolated node to G . Consider the following two conjectures.

Conjecture 1.3 ([12]). *For any graph G , we have $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G)$.*

Conjecture 1.4. *For any graph G , $\vartheta\text{-rank}(G) < \infty$ implies $\vartheta\text{-rank}(G \oplus i_0) < \infty$.*

Conjecture 1.3 is in fact posed in [12] in a more general form (see [12, Conjecture 4]). In addition, it is shown in [12] that Conjecture 1.3 implies Conjecture 1.1. We will show that Conjecture 1.4 is in fact equivalent to Conjecture 1.2 (see Proposition 4.6). In an attempt to relate $\vartheta\text{-rank}(G \oplus i_0)$ and $\vartheta\text{-rank}(G)$ let us consider the following decomposition of the graph matrices, proposed in [12], where we set $\alpha := \alpha(G)$ so that $\alpha(G \oplus i_0) = \alpha + 1$:

$$M_{G \oplus i_0} = \begin{pmatrix} \alpha & & -1 \\ -1 & (\alpha + 1)(I + A_G) & -J \end{pmatrix} = \begin{pmatrix} \alpha & -1 \\ -1 & \frac{1}{\alpha}J \end{pmatrix} + \frac{\alpha + 1}{\alpha} \begin{pmatrix} 0 & 0 \\ 0 & \alpha(I + A_G) - J \end{pmatrix}. \quad (1.8)$$

If the operation of adding a zero row/column preserves membership in the cones $\mathcal{K}^{(r)}$ then, in view of (1.8), it would immediately follow that $M_G \in \mathcal{K}_n^{(r)}$ implies $M_{G \oplus i_0} \in \mathcal{K}_{n+1}^{(r)}$, which would show Conjecture 1.3 (and thus also Conjecture 1.1). In addition, if adding a zero row/column preserves membership in the union $\bigcup_{r \in \mathbb{N}} \mathcal{K}^{(r)}$, then again in view of (1.8), Conjecture 1.4 would be true and thus Conjecture 1.2 too. However, adding a zero row/column does *not* in general preserve membership in the cones $\mathcal{K}^{(r)}$ for a given order $r \geq 1$ (while this is clearly true for order $r = 0$); this was observed (numerically) for order $r = 1$ using the graph matrix $M_{C_5} \in \mathcal{K}_5^{(1)}$ of the 5-cycle (see [5]). We will show that also the second property fails: adding a zero row/column to a matrix $M \in \bigcup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ produces a matrix that does not belong to the union $\bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+1}^{(r)}$ (see Theorem 3.2).

Motivated by the above observations, our focus in this paper is to investigate the following topics: the impact of adding a zero row/column to a matrix in $\bigcup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ (in Section 3), the behaviour of the ϑ -rank under some simple graph operations in relation to Conjectures 1.1 and 1.2 (in Section 4), structural properties of the graphs with $\vartheta\text{-rank}(G) = 0$ (in Section 5), and the impact of adding an isolated node to a graph G with $\vartheta\text{-rank}(G) = 1$ (in Section 6). We now give some more details about the last two topics.

Graphs with small ϑ -rank 0 or 1. In order to investigate the graphs with small $\vartheta\text{-rank}(G) = 0$ or 1 we will use the explicit characterizations of the cones $\mathcal{K}_n^{(0)}$ and $\mathcal{K}_n^{(1)}$ provided by Parrilo [24]. There it is shown that a matrix $M \in \mathcal{S}^n$ belongs to $\mathcal{K}_n^{(0)}$ if and only if M admits a decomposition $M = P + N$ with $P \succeq 0$, $N \geq 0$ and $N_{ii} = 0$ for all $i \in [n]$; we call such matrix P a $\mathcal{K}^{(0)}$ -certificate for M . This in particular permits to show that the bound $\vartheta^{(0)}(G)$ coincides with the bound $\vartheta'(G)$, which is the Lovasz' theta number strenghtened by adding a nonnegativity constraint (see [5]). Parrilo [24] also showed that $M \in \mathcal{K}_n^{(1)}$ if and only if there exist positive semidefinite matrices $P(1), P(2), \dots, P(n)$ satisfying certain linear constraints (see Lemma 2.2); we say that such matrices form a $\mathcal{K}^{(1)}$ -certificate for M . We exploit the structure of the zeros of the quadratic form $x^T M x$ to obtain information about the kernels of $\mathcal{K}^{(0)}$ - and $\mathcal{K}^{(1)}$ -certificates for M . This information plays a crucial role in our study of the graphs with $\vartheta\text{-rank}(G) = 0$ or 1, i.e, for which M_G belongs to $\mathcal{K}_n^{(0)}$ or $\mathcal{K}_n^{(1)}$. In some cases it permits to show uniqueness of the certificates, a useful property for the study of the ϑ -rank. As an example, the graph matrix M_{C_5} of the 5-cycle has a unique $\mathcal{K}^{(1)}$ -certificate and this uniqueness property permits to characterize the diagonal scalings of M_{C_5} that belong to $\mathcal{K}_5^{(1)}$ (see Section 3.2).

Our main results are as follows. We characterize the critical graphs with ϑ -rank 0 as the disjoint unions of cliques, and we reduce the problem of deciding whether a graph has ϑ -rank 0 to the same problem for the class of acritical graphs (see Section 5). This reduction can be done in polynomial time for the class of graphs G with fixed value of $\alpha(G)$. In addition we show that adding an isolated node to a graph with ϑ -rank 1 may produce a graph with ϑ -rank at least 2, thus disproving Conjecture 1.3 above. We also characterize the maximum number of isolated nodes that can be added to some graphs with ϑ -rank 1 (such as odd cycles and their complements) while preserving the ϑ -rank 1 property (see Section 6). For example, for the graph C_5 this maximum number of nodes is shown to be equal to 8. Here too we will exploit uniqueness properties of some of the matrices arising in $\mathcal{K}^{(1)}$ -certificates.

The study of the graphs with ϑ -rank 0 is also relevant to the question of understanding when the basic semidefinite relaxation (also known as the Shor relaxation) of a quadratic (or, more generally, polynomial) optimization problem is exact. This question has received increased attention in the recent years. We refer, e.g., to the works [2, 11, 32] (and references therein), which investigate this question for various classes of quadratic problems, such as random instances in [2] and standard quadratic programs in [11]. In fact, thanks to a reformulation of $\alpha(G)$ as the optimum value of a suitable polynomial optimization problem (involving degree $2r + 2$ forms), it turns out that the parameter $\vartheta^{(r)}(G)$ can also be viewed as the optimum value of the Shor relaxation of this polynomial optimization problem (see [12, Section 6.3]). Hence, also Conjectures 1.1 and 1.2 can be seen in the light of understanding exactness of Shor relaxations.

Yet another motivation for the study of the graphs with ϑ -rank 0 comes from its relevance to fundamental questions in complexity theory. Deciding whether a graph G has ϑ -rank(G) = 0 indeed amounts to deciding whether the polynomial $F_G(x) = (x^{o_2})^T M_G x^{o_2}$ is a sum of squares, i.e., whether an associated semidefinite program is feasible. Equivalently, as mentioned above, ϑ -rank(G) = 0 if and only if there exists a positive semidefinite matrix $P \in \mathcal{S}^n$ satisfying the linear constraints: $P_{ii} = \alpha(G) - 1$ for $i \in V$ and $P_{i,j} \leq -1$ for $\{i, j\} \notin E$, which thus again asks about the feasibility of a semidefinite program. Recall that the complexity status of deciding feasibility of a semidefinite program is still unknown. On the positive side it was shown in [27] that one can test feasibility of a semidefinite program involving matrices of size n and with m linear constraints in polynomial time when n or m is fixed. In addition, it was shown in [28] that this problem belongs to the class NP if and only if it belongs to co-NP. Understanding the complexity status for the class of semidefinite programs related to the question of testing whether ϑ -rank(G) = 0 offers a rich playground to be explored later.

Organization of the paper. The paper is organized as follows. In Section 2 we group some preliminary results. In particular, we recall the characterization of the cones $\mathcal{K}_n^{(0)}$ and $\mathcal{K}_n^{(1)}$ from [24] and we give some structural properties of the matrices arising in $\mathcal{K}^{(0)}$ - and $\mathcal{K}^{(1)}$ -certificates for membership in these cones. We also recall a characterization for the minimizers of the Motzkin-Straus formulation (2.8) for $\alpha(G)$. In Section 3, we provide explicit constructions showing that adding a zero row/column to a matrix in $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ may produce a matrix in $\text{COP}_{n+1} \setminus \bigcup_{r \geq 0} \mathcal{K}_{n+1}^{(r)}$, thereby showing strict inclusion $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subset \text{COP}_n$ for any $n \geq 6$. We also construct copositive matrices with an all-ones diagonal that do not belong to any cone $\mathcal{K}_n^{(r)}$ for $n \geq 7$, thereby disproving a conjecture from [7]. Exploiting the fact that the graph matrix M_{C_5} admits a unique $\mathcal{K}^{(1)}$ -certificate, we can characterize the diagonal scalings of M_{C_5} that still belong to $\mathcal{K}_5^{(1)}$. In Section 4 we present some known and new results dealing with the behavior on the ϑ -rank under simple graph operations like adding an isolated node and deleting an acritical edge, and we investigate their relevance for Conjectures 1.1 and 1.2. In Section 5 we discuss the role of critical edges in the study of the graphs with ϑ -rank 0. In particular, we characterize the critical graphs with ϑ -rank 0 and we give an algorithmic procedure that reduces the problem of deciding whether a graph has ϑ -rank 0 to the same problem restricted to graphs with no critical edges. In Section 6 we develop some tools using criticality (as well as symmetry and kernel properties) to study the impact of adding isolated nodes to graphs with ϑ -rank 1. As an application we can characterize how many isolated nodes can be added to an odd cycle (or its complement) while preserving the ϑ -rank 1 property. As a byproduct, we show that adding an isolated node can increase the ϑ -rank, thereby refuting Conjecture 1.3.

Notation. Given a graph $G = (V, E)$, a set $S \subseteq V$ is stable (aka independent) if S does not contain any edge of G . Then, $\alpha(G)$ denotes the maximum cardinality of a stable set, called the *stability number* of G . For a subset $U \subseteq V$, $G[U]$ denotes the induced subgraph of G , with vertex set U and edge set $\{\{i, j\} \in E : i, j \in U\}$ and, given an edge $e \in E$, $G \setminus e = (V, E \setminus \{e\})$ is the subgraph obtained by deleting the edge e . An edge $e \in E$ is *critical* if $\alpha(G \setminus e) = \alpha(G) + 1$ and e is called *acritical* otherwise. We say that G is *critical* if all its edges are critical and that G is *acritical* if it has no critical edges. A set $C \subseteq V$ is a clique if $\{i, j\} \in E$ for all $i \neq j \in C$ and the maximum cardinality of a clique is $\omega(G) = \alpha(\overline{G})$. Then $\chi(G)$ (resp., $\chi(\overline{G})$) denotes the minimum number of stable sets (resp., cliques) whose union is V . For convenience we also set $\overline{\chi}(G) = \chi(\overline{G})$. Clearly one has $\omega(G) \leq \chi(G)$ and $\alpha(G) \leq \overline{\chi}(G)$. Recall that a graph G is called *perfect* if $\chi(H) = \omega(H)$ for every induced subgraph H of G . The celebrated *strong perfect graph theorem* of Chudnovsky et al. [3] shows that G is perfect if and only if G does not contain an odd cycle C_{2n+1} or its complement \overline{C}_{2n+1} ($n \geq 2$) as an induced subgraph. For a node $i \in V$, $N(i)$ denotes the set of nodes $j \in V$ that are adjacent to i and $i^\perp := \{i\} \cup N(i)$ is the closed neighborhood of i ; then i is called an isolated node if $N(i) = \emptyset$. For a subset $S \subseteq V$ set $N_S(i) = N(i) \cap S$. For a graph G and a node $i_0 \notin V$, $G \oplus i_0 = (V \cup \{i_0\}, E)$ denotes the graph obtained by adding the isolated node i_0 to G . In general, given two graphs G and H , the graph $G \oplus H = (V(G) \cup V(H), E(G) \cup E(H))$ denotes the disjoint union of G and H .

We let \mathcal{S}^n denote the set of $n \times n$ symmetric matrices. For a matrix $M \in \mathcal{S}^n$, we write $M \succeq 0$ if it is positive semidefinite (i.e., $x^T M x \geq 0$ for all $x \in \mathbb{R}^n$) and $M \geq 0$ if all its entries are nonnegative. For a set $S \subseteq [n]$, $M[S]$ denotes the principal submatrix of M whose rows and columns are indexed by S . Throughout J_n, I_n denote the all-ones matrix and the identity matrix of size n and we may omit the subscript n when the size is not important or clear from the context. For integers $m, n \geq 1$, $J_{m,n}$ denotes the $m \times n$ all-ones matrix. Throughout e denotes the all-ones vector (of appropriate size). For a vector $x \in \mathbb{R}^n$, $\text{Supp}(x) = \{i \in [n] : x_i \neq 0\}$ denotes its support. The adjacency matrix $A_G \in \mathcal{S}^n$ of a graph $G = (V = [n], E)$ has entries $(A_G)_{ij} = 1$ if $\{i, j\} \in E$ and zero otherwise.

Throughout $\mathbb{R}[x] = \mathbb{R}[x_1, \dots, x_n]$ denotes the set of n -variate polynomials and Σ is the set of sums of squares of polynomials, i.e., of the form $p_1^2 + \dots + p_m^2$ for some $m \in \mathbb{N}$ and $p_1, \dots, p_m \in \mathbb{R}[x]$. The degree of a polynomial $f \in \mathbb{R}[x]$ is the largest degree d of its terms and f is said to be homogeneous of degree d if all its terms have degree d .

2 Preliminaries on the cones $\mathcal{K}_n^{(r)}$

Recall that the cone $\mathcal{K}_n^{(r)}$ consists of the matrices $M \in \mathcal{S}^n$ for which the polynomial $(\sum_{i=1}^n x_i^2)^r ((x^{\circ 2})^T M x^{\circ 2})$ is a sum of squares of polynomials. A useful characterization for matrices in $\mathcal{K}_n^{(r)}$ is given by the following general result.

Theorem 2.1 (Peña et al. [31]). *Let $q \in \mathbb{R}[x]$ be a homogeneous polynomial of degree d and define the degree $2d$ polynomial $Q(x) := q(x^{\circ 2}) = q(x_1^2, \dots, x_n^2)$. Then, $Q \in \Sigma$ if and only if q can be decomposed as*

$$q(x) = \sum_{\substack{I \subseteq [n] \\ |I| \leq d, |I| \equiv d \pmod{2}}} \sigma_I(x) \prod_{i \in I} x_i, \quad (2.1)$$

where σ_I is a homogeneous polynomial with degree $d - |I|$ and $\sigma_I \in \Sigma$.

As an application, $M \in \mathcal{K}_n^{(0)}$ if and only if there exist a matrix $P \succeq 0$ and scalars $c_{ij} \geq 0$ for $1 \leq i < j \leq n$ such that

$$x^T M x = x^T P x + \sum_{0 \leq i < j \leq n} c_{ij} x_i x_j. \quad (2.2)$$

This corresponds to the characterization of the cone $\mathcal{K}_n^{(0)}$ given by Parrilo in [24], which reads

$$\mathcal{K}_n^{(0)} = \{P + N : P \succeq 0, N \geq 0\}. \quad (2.3)$$

Note that in (2.3) we can indeed assume, without loss of generality, that $N_{ii} = 0$ for all $i \in [n]$. We say that P is a $\mathcal{K}^{(0)}$ -certificate for M if $P \succeq 0$, $P \leq M$ and $P_{ii} = M_{ii}$ for all $i \in [n]$. In other words, P is a $\mathcal{K}^{(0)}$ -certificate for M if there exist scalars $c_{ij} \geq 0$ for $1 \leq i < j \leq n$ for which Eq. (2.2) holds.

Similarly, using Theorem 2.1, $M \in \mathcal{K}_n^{(1)}$ if and only if there exist matrices $P(i) \succeq 0$ for $i \in [n]$ and scalars $c_{ijk} \geq 0$ for distinct $i, j, k \in [n]$ such that

$$\left(\sum_{i=1}^n x_i \right) x^T M x = \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k. \quad (2.4)$$

From this, we get the characterization of the cone $\mathcal{K}_n^{(1)}$ from Parrilo [24] (see also [5]).

Lemma 2.2. *A matrix M belongs to the cone $\mathcal{K}_n^{(1)}$ if and only if there exist matrices $P(i) \succeq 0$ for $i \in [n]$ and scalars $c_{ijk} \geq 0$ for $1 \leq i < j < k \leq n$ satisfying Equation (2.4). Equivalently, there exist matrices $P(i) \in \mathcal{S}^n$ for $i \in [n]$ satisfying the following conditions:*

- (i) $P(i) \succeq 0$ for all $i \in [n]$,
- (ii) $P(i)_{ii} = M_{ii}$ for all $i \in [n]$,
- (iii) $2P(i)_{ij} + P(j)_{ii} = 2M_{ij} + M_{ii}$ for all $i \neq j \in [n]$,
- (iv) $P(i)_{jk} + P(j)_{ik} + P(k)_{ij} \leq M_{ij} + M_{ik} + M_{jk}$ for all distinct $i, j, k \in [n]$.

Proof. As observed above, $M \in \mathcal{K}_n^{(1)}$ if and only if there exist matrices $P(i) \succeq 0$ for $i \in [n]$ and scalars $c_{ijk} \geq 0$ satisfying Eq.(2.4). We now obtain the conditions (ii)-(iv) by comparing coefficients at both sides of (2.4). We give the details since they will be useful later. First, we start with the left hand side in (2.4):

$$\left(\sum_{i=1}^n x_i \right) x^T M x = \sum_{i=1}^n M_{ii} x_i^3 + \sum_{i \neq j \in [n]} x_i^2 x_j (M_{ii} + 2M_{ij}) + \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (M_{ij} + M_{jk} + M_{ik}). \quad (2.5)$$

Now we expand the right hand side in (2.4):

$$\begin{aligned} & \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k \\ &= \sum_{i=1}^n x_i^3 P(i)_{ii} + \sum_{i \neq j \in [n]} x_i^2 x_j (P(j)_{ii} + 2P(i)_{ij}) + \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (P(i)_{jk} + P(j)_{ik} + P(k)_{ij} + c_{ijk}). \end{aligned} \quad (2.6)$$

Comparing coefficients at both sides we obtain the desired result. \square

Remark 2.3. Observe that Lemma 2.2 remains valid if in (i) we replace the condition $P(i) \succeq 0$ by the weaker condition $P(i) \in \mathcal{K}_n^{(0)}$. Indeed, as $\mathcal{K}_n^{(0)} = \mathcal{S}_+^n + \mathbb{R}_+^{n \times n}$, the ‘only if’ part is clear since $\mathcal{S}_+^n \subseteq \mathcal{K}_n^{(0)}$, and the ‘if part’ follows easily from the fact that $(x^{\circ 2})^T N x^{\circ 2} \in \Sigma$ for any $N \in \mathbb{R}_+^{n \times n}$.

We say that the matrices $P(1), P(2), \dots, P(n)$ are a $\mathcal{K}^{(1)}$ -certificate for M if they satisfy the conditions (i)-(iv) of Lemma 2.2. In other words, the matrices $P(1), \dots, P(n)$ are a $\mathcal{K}^{(1)}$ -certificate of M if they are positive semidefinite and there exist scalars $c_{ijk} \geq 0$ for $1 \leq i < j < k \leq n$ satisfying Eq. (2.4).

Now we give some easy, but crucial properties of $\mathcal{K}^{(0)}$ - and $\mathcal{K}^{(1)}$ -certificates, involving their kernel, that will be repeatedly used in the paper.

Lemma 2.4. Let $M \in \mathcal{K}_n^{(0)}$ and let P be a $\mathcal{K}^{(0)}$ -certificate of M . If $x \in \mathbb{R}_+^n$ and $x^T M x = 0$, then $Px = 0$ and $P[S] = M[S]$, where $S = \{i \in [n] : x_i > 0\}$ is the support of x .

Proof. Since P is a $\mathcal{K}^{(0)}$ -certificate there exists a matrix $N \geq 0$ such that $M = P + N$. Hence, $0 = x^T M x = x^T P x + x^T N x$. Then $x^T P x = 0 = x^T N x$ as $P \succeq 0$ and $N \geq 0$. This implies $Px = 0$ since $P \succeq 0$. On the other hand, since $x^T N x = 0$ and $N \geq 0$, we get $N_{ij} = 0$ for $i, j \in S$. Hence, $M[S] = P[S]$, as $M = P + N$. \square

Lemma 2.5. Let $M \in \mathcal{K}_n^{(1)}$ and let $P(1), \dots, P(n)$ be a $\mathcal{K}^{(1)}$ -certificate of M . Let $x \in \mathbb{R}_+^n$ such that $x^T M x = 0$. Then the following holds:

- (i) If $x_i > 0$ then $P(i)x = 0$.
- (ii) If $x_i, x_j, x_k > 0$ then $M_{ij} + M_{jk} + M_{ik} = P(i)_{ij} + P(j)_{ik} + P(k)_{ij}$.

Proof. By evaluating Eq. (2.4) at x , we get that the left hand side is zero while all terms in the right hand side are nonnegative, so all of them vanish. Hence, if $x_i > 0$ then $x^T P(i)x = 0$, which implies $P(i)x = 0$ as $P(i) \succeq 0$. On the other hand, if $x_i x_j x_k > 0$ then $c_{ijk} = 0$, which implies the desired identity (see Eq. (2.5) and Eq. (2.6)). \square

Example 2.6. Consider the 5-cycle C_5 shown in Fig. 1 and the associated graph matrix $M_{C_5} = 2(A_{C_5} + I) - J$, also known as the Horn matrix and denoted by H .

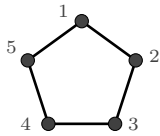


Figure 1: Graph C_5

$$H = M_{C_5} = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{pmatrix}$$

The Horn matrix

The Horn matrix H is known to belong to $\mathcal{K}_n^{(1)}$ [24]. As we now show, it admits a unique $\mathcal{K}^{(1)}$ -certificate, where the matrices $P(1), \dots, P(5)$ are of the form shown below:

$$P(1) = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 \end{pmatrix}, \quad P(i) = \begin{pmatrix} \overbrace{1 & 1 & 1}^{i^\perp} & \overbrace{-1 & -1}^{V \setminus i^\perp} \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 \end{pmatrix} \quad \text{for } i \in [5]. \quad (2.7)$$

Up to symmetry it suffices to show that $P(1)$ has the above shape. Let C_1, C_2, C_3, C_4, C_5 denote its columns. Since the vectors $(1, 0, 1, 0, 0)$, $(1, 0, 0, 1, 0)$, $(1, 1, 0, 2, 0)$, $(1, 0, 2, 0, 1)$ are zeros of the form $x^T H x$, by Lemma 2.5 (i), we obtain $C_1 = -C_3$, $C_1 = -C_4$, $C_1 + C_2 + 2C_4 = 0$ and $C_1 + C_5 + 2C_3 = 0$. Hence, $C_1 = C_2 = C_5 = -C_3 = -C_4$. Since $P(1)_{11} = 1$ the above conditions determine the first row and column and therefore the rest of the matrix $P(1)$, which thus has the desired shape.

As shown in the previous lemmas, the zeros of the quadratic form $x^T M x$ give us information about the kernel of $\mathcal{K}^{(0)}$ - and $\mathcal{K}^{(1)}$ -certificates for M . For the case of the graph matrices $M_G = \alpha(G)(A_G + I) - J$ there is a full characterization of the zeros of this quadratic form in Δ_n (and thus in \mathbb{R}_+^n). First, observe that, for $x \in \Delta_n$, we have $x^T M_G x = 0$ if and only if x is an optimal solution of the following program

$$\frac{1}{\alpha(G)} = \min\{x^T (I + A_G)x : x \in \Delta_n\}. \quad (2.8)$$

Indeed we have

$$x^T M_G x = 0 \iff \alpha(G) x^T (A_G + I) x - x^T J x = 0 \iff x^T (A_G + I) x = \frac{1}{\alpha(G)}. \quad (2.9)$$

The formulation of $\alpha(G)$ in (2.8) is due to Motzkin and Straus [23] and underlies its copositive formulation in (1.1).

We conclude with recalling the characterization of the minimizers of problem (2.8), following [19, Corollary 4.4] (see also [10]).

Theorem 2.7. *Let $x \in \Delta_n$ with support $S = \{i \in [n] : x_i > 0\}$, and let V_1, V_2, \dots, V_k denote the connected components of the graph $G[S]$. Then x is an optimal solution of (M-S) if and only if $k = \alpha(G)$, V_i is a clique and $\sum_{j \in V_i} x_j = \frac{1}{\alpha(G)}$ for all $i \in [k]$. In that case all edges in $G[S]$ are critical edges of G .*

3 On the exactness of the approximation of COP_n by the Parrilo cones $\mathcal{K}_n^{(r)}$

In this section we investigate the cones $\mathcal{K}_n^{(r)}$, which were introduced by Parrilo [24] as inner approximations of the copositive cone COP_n and satisfy

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n.$$

As pointed out in [5, 12], one difficulty for the understanding of the cones $\mathcal{K}_n^{(r)}$ is that they are not closed under adding a zero row/column when $r \geq 1$. In addition, while $\text{COP}_4 = \mathcal{K}_4^{(0)}$, it is shown in [7] that for any $n \geq 5$ the copositive cone COP_n is not contained in a single cone $\mathcal{K}_n^{(r)}$ for any $r \in \mathbb{N}$. Here we prove that the situation is even worse: for $n \geq 6$, the cone COP_n is not even contained in the union of the cones $\mathcal{K}_n^{(r)}$. For this, we show that if a copositive matrix does not belong to the cone $\mathcal{K}_n^{(0)}$ then after adding to it a zero row/column the resulting matrix does not belong to any of the cones $\mathcal{K}_{n+1}^{(r)}$ ($r \geq 0$). The question of whether the union of the cones $\mathcal{K}_5^{(r)}$ covers the full copositive cone COP_5 remains open. Motivated by this question one may ask whether any diagonal scaling of the Horn matrix $H = M_{C_5}$ lies in some cone $\mathcal{K}_5^{(r)}$. We will characterize the diagonal scalings of H that belong to the cone $\mathcal{K}_5^{(1)}$, which crucially relies on the fact that H admits a unique $\mathcal{K}^{(1)}$ -certificate.

3.1 Constructing copositive matrices not belonging to any Parrilo cone

Dickinson et al. [7] conjectured that for any integer $n \geq 1$ there exists an integer $r \geq 0$ such that any copositive matrix of size n with 0, 1-valued diagonal entries lies in the cone $\mathcal{K}_n^{(r)}$. The conjecture holds for $n \leq 4$ with $r = 0$ since $\text{COP}_4 = \mathcal{K}_4^{(0)}$. For $n = 5$ it is shown in [7] that the conjecture holds with $r = 1$. Here we will show that this conjecture does not hold for $n \geq 6$. Even more we give an example of copositive matrix with an all-ones diagonal that does not belong to any of the cones $\mathcal{K}_n^{(r)}$. For this, we consider the following construction. Given two copositive matrices $M_1 \in \text{COP}_n$ and $M_2 \in \text{COP}_m$, we consider their direct sum

$$M_1 \oplus M_2 := \left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array} \right), \quad (3.1)$$

which is clearly copositive. We will show below that, under some conditions on M_1, M_2 , the matrix $M_1 \oplus M_2$ does not belong to any of the cones $\mathcal{K}_{n+m}^{(r)}$. We start with a preliminary result on sums of squares of polynomials.

Lemma 3.1. *Let f be a polynomial of degree $2d$ in n variables. Write $f = f_r + f_{r+1} + \dots + f_{2d}$ where $f_r \neq 0$ and, for $r \leq j \leq 2d$, each f_j is a homogeneous polynomial with degree j . If f is a sum of squares then f_r is a sum of squares.*

Proof. Since f is a sum of squares we have $f = \sum_{i=1}^m q_i^2$ for some $q_i \in \mathbb{R}[x]$ with $\deg(q_i) \leq d$ for all $i \in [m]$. Then each q_i has the form $q_i = \sum_{j=0}^d a_i^{(j)}$, where each nonzero $a_i^{(j)}$ is a homogeneous polynomial of degree j . For $i \in [m]$ set $L_i = \min\{j : a_i^{(j)} \neq 0\}$ and set $L = \min\{L_i : i \in [m]\}$. Notice that there is no monomial with degree less than $2L$ in $\sum_i q_i^2 = f$ and $f_{2L} = \sum_{i=1}^m (a_i^{(L)})^2 \neq 0$. Hence it follows that $f_r = f_{2L}$ is a sum of squares. \square

Theorem 3.2. *Let $M_1 \in \text{COP}_n$ and $M_2 \in \text{COP}_m$ be two copositive matrices. Assume that $M_1 \notin \mathcal{K}_n^{(0)}$ and that there exists $0 \neq z \in \mathbb{R}_+^m$ such that $z^T M_2 z = 0$. Then we have*

$$\left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array} \right) \in \text{COP}_{n+m} \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+m}^{(r)}. \quad (3.2)$$

Proof. Assume for contradiction $M_1 \oplus M_2 \in \mathcal{K}_n^{(r)}$, i.e., the polynomial $(p_{M_1}(x) + p_{M_2}(y))(\sum_{i=1}^n x_i^2 + \sum_{j=1}^m y_j^2)^r$ is a sum of squares. Here, for convenience, we denote the $n + m$ variables as x_i ($i \in [n]$) and y_j ($j \in [m]$) and we set $p_{M_1}(x) = (x^{\circ 2})^T M_1 x^{\circ 2}$ and $p_{M_2}(y) = (y^{\circ 2})^T M_2 y^{\circ 2}$. Write $z = y^{\circ 2}$ for some $y \in \mathbb{R}^m$, so that $p_{M_2}(y) = 0$, and $c := \sum_{j=1}^m y_j^2 > 0$. Then the polynomial $f(x) := p_{M_1}(x)(\sum_{i=1}^n x_i^2 + c)^r$ is a sum of squares. By decomposing f as a sum of homogeneous polynomials we see that its least degree homogeneous part is the polynomial $cp_{M_1}(x)$, with degree 4. By Lemma 3.1 we obtain that $cp_{M_1}(x)$ is a sum of squares, i.e, $M_1 \in \mathcal{K}_n^{(0)}$, yielding a contradiction. \square

We now use Theorem 3.2 to give some classes of copositive matrices that do not belong to $\mathcal{K}^{(r)}$ for any $r \in \mathbb{N}$. As a first application we obtain

$$M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)} \implies \left(\begin{array}{c|c} M & 0 \\ \hline 0 & 0 \end{array} \right) \in \text{COP}_{n+1} \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+1}^{(r)}. \quad (3.3)$$

Since the inclusion $\mathcal{K}_5^{(0)} \subset \text{COP}_5$ is strict this shows that also the inclusion $\bigcup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)} \subset \text{COP}_n$ is strict for any $n \geq 6$. Hence the cone $\bigcup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)}$ is not a closed set for $n \geq 6$. On the other hand, we have $\text{COP}_n = \mathcal{K}_n^{(0)}$ for $n \leq 4$ [6]. The situation for the case of 5×5 matrices remains open.

Question 3.3. Does equality $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ hold?

Dickinson et al. [7] proved that any 5×5 copositive matrix with 0,1-valued diagonal entries belongs to $\mathcal{K}_5^{(1)}$. They conjectured that for any integer $n \geq 6$ there exists an integer $r \geq 0$ such that any $n \times n$ copositive matrix with 0,1-valued diagonal entries belongs to $\mathcal{K}_n^{(r)}$ (see [7, Conjecture 1]). Using Theorem 3.2 we can disprove this conjecture.

Example 3.4. Let $M_1 := M_{C_5} = H$ be the Horn matrix, known to be copositive with $H \notin \mathcal{K}_5^{(0)}$. For the matrix M_2 we first consider the 1×1 matrix $M_2 = 0$ and as a second example we consider $M_2 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \in \text{COP}_2$. Then, as an application of Theorem 3.2, we obtain

$$\left(\begin{array}{c|c} H & 0 \\ \hline 0 & 0 \end{array} \right) \in \text{COP}_6 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_6^{(r)}, \quad \left(\begin{array}{c|cc} H & & 0 \\ \hline 0 & 1 & -1 \\ & -1 & 1 \end{array} \right) \in \text{COP}_7 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_7^{(r)}. \quad (3.4)$$

The left most matrix in (3.4) is copositive, has all its diagonal entries equal to 0,1 and does not belong to any of the cones $\mathcal{K}_6^{(r)}$; selecting for M_2 the zero matrix of size $m \geq 1$ gives a matrix in $\text{COP}_n \setminus \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ for any size $n \geq 6$. The right most matrix in (3.4) is copositive, has all its diagonal entries equal to 1 and does not lie in any of the cones $\mathcal{K}_7^{(r)}$. More generally, if we select the matrix $M_2 = \frac{1}{m-1}(mI_m - J_m)$, which is positive semidefinite with $e^T M_2 e = 0$, then we obtain a matrix in $\text{COP}_n \setminus \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ with diagonal entries equal to 1, for any size $n \geq 7$. In contrast, as mentioned above, Dickinson et al. [7] proved that any copositive 5×5 matrix with an all-ones diagonal belongs to $\mathcal{K}_5^{(1)}$. The situation for the case of 6×6 copositive matrices remains open.

Question 3.5. Is it true that any 6×6 copositive matrix with an all-ones diagonal belongs to $\mathcal{K}_6^{(r)}$ for some $r \in \mathbb{N}$?

We conclude with an observation on the number of zeros in the simplex Δ_n of the quadratic form $x^T M x$ when M is a copositive matrix. For the class of copositive matrices arising from the graph matrices $M_G = \alpha(G)(A_G + I) - J$ it is proved in [19] that the number of such zeros is finite if and only if the graph G is acritical, in which case the matrix M_G belongs to some cone $\mathcal{K}^{(r)}$. We now show that the property of having finitely many zeros in the simplex for the quadratic form $x^T M x$ is in general not sufficient to ensure membership of M in some cone $\mathcal{K}^{(r)}$. Specifically, we give a class of copositive matrices $M \notin \bigcup_r \mathcal{K}^{(r)}$ for which the quadratic form $x^T M x$ has a unique zero in Δ_n .

Example 3.6. Let $M_1 \in \text{COP}_n$ be a strictly copositive matrix such that $M_1 \notin \mathcal{K}_n^{(0)}$. For instance, one can take $M_1 = t(I + A_G) - J$, where G is a graph with $\vartheta\text{-rank}(G) \geq 1$ and $\alpha(G) < t < \vartheta^{(0)}(G)$. By Theorem 3.2 we have

$$M := \left(\begin{array}{c|cc} M_1 & & 0 \\ \hline 0 & 1 & -1 \\ & -1 & 1 \end{array} \right) \in \text{COP}_{n+2} \setminus \bigcup_{r \geq 0} \mathcal{K}_{n+2}^{(r)}. \quad (3.5)$$

Now we prove that the quadratic form $x^T M x$ has a unique zero in the simplex. For this let $x \in \Delta_{n+2}$ such that $x^T M x = 0$. Since M_1 is strictly copositive and $y := (x_1, \dots, x_n)$ is a zero of the quadratic form $y^T M_1 y$ it follows

that $x_1 = \dots = x_n = 0$. Hence (x_{n+1}, x_{n+2}) is a zero of the quadratic form $x_{n+1}^2 - 2x_{n+1}x_{n+2} + x_{n+2}^2$ in the simplex Δ_2 and thus $x_{n+1} = x_{n+2} = 1/2$. This shows that the only zero of the quadratic form $x^T Mx$ in the simplex is $(0, 0, \dots, 0, \frac{1}{2}, \frac{1}{2})$, as desired.

3.2 Characterizing the diagonal scalings of the Horn matrix in $\mathcal{K}^{(1)}$

As mentioned above, it is not known whether the union of the cones $\mathcal{K}_5^{(r)}$ covers the full cone COP_5 , but any matrix in COP_5 with 0, 1-valued diagonal entries lies in the cone $\mathcal{K}_5^{(1)}$ [7]. One of the key ingredients for this result is the complete characterization of the extreme rays of the cone COP_5 by Hildebrand [14]. In particular the Horn matrix H and its positive diagonal scalings define a class of extreme rays of COP_5 , so the question arises whether all of them lie in some cone $\mathcal{K}_5^{(r)}$. Here, a positive diagonal scaling of a matrix M is a matrix of the form DMD , where $D = \text{diag}(d_1, \dots, d_5)$ with $d_1, \dots, d_5 > 0$.

Question 3.7. *Is it true that every positive diagonal scaling of the Horn matrix belongs to $\mathcal{K}_5^{(r)}$ for some r ?*

As a first partial step we characterize the diagonal scalings of the Horn matrix that lie in $\mathcal{K}_5^{(1)}$. A key ingredient for this is the fact that the Horn matrix admits a unique $\mathcal{K}^{(1)}$ -certificate, as was observed in Example 2.6.

Theorem 3.8. *Let $D = \text{diag}(d_1, d_2, d_3, d_4, d_5)$ with $d_1, \dots, d_5 > 0$ and let H be the Horn matrix. Then, DHD belongs to $\mathcal{K}_5^{(1)}$ if and only if d_1, \dots, d_5 satisfy the following inequalities*

$$d_{i-1}d_i + d_i d_{i+1} \geq d_{i-1}d_{i+1} \text{ for } i \in [5] \text{ (indices taken modulo 5)}. \quad (3.6)$$

Proof. Set $M := DHD$. First we show the ‘if part’. Assume d_1, \dots, d_5 satisfy conditions (3.6); we show $M \in \mathcal{K}_5^{(1)}$. For this consider the matrices $Q(i) := DP(i)D$, where the matrices $P(i)$ are the $\mathcal{K}^{(1)}$ -certificate for H from (2.7); we show that the matrices $Q(i)$ form a $\mathcal{K}^{(1)}$ -certificate for M , i.e., satisfy the conditions (i)-(iv) from Lemma 2.2. Clearly $Q(i) \geq 0$ and $Q(i)_{ii} = d_i^2$ for all $i \in [5]$, so (i), (ii) hold. Also, $2Q(i)_{ij} + Q(j)_{ii} = 2d_i d_j P(i)_{ij} + d_j^2 P(j)_{ii} = 2M_{ij} + M_{ii}$ since $P(i)_{ij} = H_{ij}$ and $P(j)_{ii} = H_{ii}$, so (iii) holds. We now check (iv), i.e., $Q(i)_{jk} + Q(j)_{ik} + Q(k)_{ij} \leq M_{ij} + M_{jk} + M_{ik}$ for any distinct $i, j, k \in [5]$. There are two possible patterns (up to symmetry): $(i, j, k) = (1, 2, 4)$ and $(i, j, k) = (5, 1, 2)$. For the first pattern we get

$$Q(1)_{24} + Q(2)_{14} + Q(4)_{12} = d_2 d_4 P(1)_{24} + d_1 d_4 P(2)_{14} + d_1 d_2 P(4)_{12} = M_{24} + M_{14} + M_{12}.$$

For the second pattern we get

$$\begin{aligned} & M_{12} + M_{25} + M_{15} - (Q(5)_{12} + Q(1)_{25} + Q(2)_{15}) \\ &= d_1 d_2 - d_2 d_5 + d_1 d_5 - (d_1 d_2 P(5)_{12} + d_2 d_5 P(1)_{25} + d_1 d_5 P(2)_{15}) \\ &= d_1 d_2 - d_2 d_5 + d_1 d_5 - (-d_1 d_2 + d_2 d_5 - d_1 d_5) \\ &= 2(d_1 d_2 - d_2 d_5 + d_1 d_5), \end{aligned}$$

which is nonnegative if and only if (3.6) holds. Hence the conditions (3.6) indeed imply that the condition (iii) of Lemma 2.2 holds for the matrices $Q(i)$ and thus they form a $\mathcal{K}^{(1)}$ -certificate for M , as desired.

Conversely, assume $M = DHD \in \mathcal{K}_5^{(1)}$ and let $Q(i)$ ($i \in [5]$) be a $\mathcal{K}^{(1)}$ -certificate for M ; we show $Q(i) = DP(i)D$ for $i \in [5]$, where the matrices $P(i)$ are the unique $\mathcal{K}^{(1)}$ -certificate for H from (2.7). In view of the above this implies that the d_i ’s satisfy the conditions (3.6), as desired. Up to symmetry it suffices to show $Q(1) = DP(1)D$. For this note that if $z^T H z = 0$ for $z \in \mathbb{R}_+^n$, then $y^T M y = 0$ for $y := D^{-1}z \in \mathbb{R}_+^n$ and thus, by Lemma 2.5, $Q(i)y = 0$ whenever $y_i > 0$. Consider the vectors $z_1 = (1, 0, 1, 0, 0)$, $z_2 = (1, 0, 0, 1, 0)$, $z_3 = (1, 1, 0, 2, 0)$, $z_4 = (1, 0, 2, 0, 1)$, which are zeros of $x^T H x$, and the corresponding vectors $y_i = D^{-1}z_i$ for $i = 1, 2, 3, 4$, which are zeros of $x^T M x$. Let C_1, \dots, C_5 denote the columns of $Q(1)$. Then, using the zeros y_1, \dots, y_5 of $x^T M x$ we obtain the relations

$$\frac{C_1}{d_1} + \frac{C_3}{d_3} = 0, \quad \frac{C_1}{d_1} + \frac{C_4}{d_4} = 0, \quad \frac{C_1}{d_1} + \frac{C_2}{d_2} + 2\frac{C_4}{d_4} = 0, \quad \frac{C_1}{d_1} + 2\frac{C_3}{d_3} + \frac{C_5}{d_5} = 0,$$

which imply $\frac{C_1}{d_1} = \frac{C_2}{d_2} = \frac{C_3}{d_3} = -\frac{C_4}{d_4} = -\frac{C_5}{d_5}$. As $Q(1)_{11} = d_1^2$ one easily deduces $Q(1) = DP(1)D$, as desired. \square

4 Behavior of the ϑ -rank under simple graph operations

Recall that the ϑ -rank of G is the minimum integer r such that $\vartheta^{(r)}(G) = \alpha(G)$. In this section, we present some useful ideas for bounding the ϑ -rank based on simple graph operations. Namely, we investigate the role of isolated

nodes and of critical edges, and their impact on Conjectures 1.1 and 1.2. In particular, we will show that it suffices to show Conjectures 1.1 and 1.2 for the class of critical graphs and that Conjecture 1.2 holds if the ϑ -rank remains finite under the operation of adding isolated nodes.

We start with a lemma relating the ϑ -rank of a graph and that of its induced subgraphs with the same stability number, which we will use later on.

Lemma 4.1. *Let $G = (V, E)$ be a graph and let H be an induced subgraph of G such that $\alpha(G) = \alpha(H)$. Then, $\vartheta\text{-rank}(H) \leq \vartheta\text{-rank}(G)$.*

Proof. As $\alpha(G) = \alpha(H) =: \alpha$ we have $M_G = \alpha(A_G + I) - J$ and $M_H = \alpha(A_H + I) - J$. As H is an induced subgraph of G , M_H is a principal submatrix of M_G and thus $M_G \in \mathcal{K}^{(r)}$ implies $M_H \in \mathcal{K}^{(r)}$. \square

Remark 4.2. *Let G be the graph obtained by adding a pendant edge to C_5 (see the left most graph in Fig. 3), so that $\alpha(G) = 3 = \alpha(C_5) + 1$. Then, G has ϑ -rank 0 as it can be covered by $\alpha(G) = 3$ cliques. However, C_5 is an induced subgraph of G and has ϑ -rank 1 (see Example 2.6). This shows that the condition of having the same stability number in Lemma 4.1 cannot be dropped.*

4.1 Role of isolated nodes

We recall a result from [12], which is useful for bounding the ϑ -rank of a graph in terms of the ϑ -rank of certain subgraphs with an added isolated node.

Proposition 4.3 ([12]). *For any graph $G = (V, E)$ we have:*

$$\vartheta\text{-rank}(G) \leq 1 + \max_{i \in V} \vartheta\text{-rank}((G \setminus i^\perp) \oplus i). \quad (4.1)$$

In view of Proposition 4.3, understanding how adding isolated nodes changes the ϑ -rank is crucial for Conjectures 1.1 and 1.2. On the one hand, it was shown in [12] that if adding an isolated node does not increase the ϑ -rank then Conjecture 1.1 holds.

Proposition 4.4 ([12]). *Assume $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G)$ for any graph G . Then Conjecture 1.1 holds.*

As we now show, if after adding an isolated node the ϑ -rank can increase by at most an absolute constant $a \in \mathbb{N}$, then we can bound $\vartheta\text{-rank}(G)$ in terms of $\alpha(G)$. In particular, when $a = 0$ we recover Proposition 4.4.

Proposition 4.5. *Let $a \in \mathbb{N}$ be a nonnegative number. Assume that $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G) + a$ for all graphs G . Then $\vartheta\text{-rank}(G) \leq (a + 1)\alpha(G) - 1$ for all graphs G .*

Proof. We proceed by induction on $\alpha(G)$. If $\alpha(G) = 1$ then $\vartheta\text{-rank}(G) = 0 \leq a$. Assume now $\alpha(G) \geq 2$. Using Proposition 4.3 and the assumption we get $\vartheta\text{-rank}(G) \leq a + 1 + \max_{i \in V} \vartheta\text{-rank}(G \setminus i^\perp)$. Since $\alpha(G \setminus i^\perp) \leq \alpha(G) - 1$, we can apply the induction assumption to $G \setminus i^\perp$ and obtain $\vartheta\text{-rank}(G \setminus i^\perp) \leq (a + 1)(\alpha(G) - 1) - 1$. This gives $\vartheta\text{-rank}(G) \leq a + 1 + (a + 1)(\alpha(G) - 1) - 1 = (a + 1)\alpha(G) - 1$. \square

On the other hand, as we now show, Conjecture 1.2 holds if and only if the ϑ -rank remains finite after adding isolated nodes to finite ϑ -rank graphs.

Proposition 4.6. *Conjecture 1.2 holds if and only if $\vartheta\text{-rank}(G) < \infty$ implies $\vartheta\text{-rank}(G \oplus i_0) < \infty$.*

Proof. The ‘only if’ part is clear. We show the ‘if’ part by contradiction. So assume that $\vartheta\text{-rank}(G) < \infty$ implies $\vartheta\text{-rank}(G \oplus i_0) < \infty$. Assume also that Conjecture 1.2 does not hold and let $G = (V, E)$ be a counterexample with the minimum number of nodes, so $\vartheta\text{-rank}(G) = \infty$. By Proposition 4.3, we obtain that $\vartheta\text{-rank}(G \setminus i^\perp \oplus i) = \infty$ for some $i \in V$. If i is not isolated in G , then $G \setminus i^\perp \oplus i$ would be a counterexample with less nodes than G , contradicting the minimality of G . Hence i is isolated in G , and thus we have $G = (G \setminus i) \oplus i$. Using again the minimality assumption, we know that $\vartheta\text{-rank}(G \setminus i) < \infty$, which implies $\vartheta\text{-rank}(G) = \vartheta\text{-rank}((G \setminus i) \oplus i) < \infty$, thus yielding a contradiction. \square

Clearly, if G has an isolated node i_0 , then $G \setminus i_0 \oplus i_0 = G$ and thus the above result in Proposition 4.3 is of no use to derive information about the ϑ -rank of G from the ϑ -rank of the graphs $G \setminus i^\perp \oplus i$. This observation (already made in [12]) points out to the difficulty of analysing the ϑ -rank of graphs with isolated nodes. We will investigate this question in Section 6.2 below.

On the other hand, adding an isolated node to a graph with ϑ -rank = 0 preserves the property of having ϑ -rank = 0. To see this, consider a graph G and set $\alpha(G) = \alpha$, so that $\alpha(G \oplus i_0) = \alpha + 1$. Then, in view of (1.8), the matrix $M_{G \oplus i_0}$ belongs to $\mathcal{K}_{n+1}^{(0)}$ if $M_G \in \mathcal{K}_n^{(0)}$. Indeed, the first matrix in the sum in (1.8) is positive semidefinite and the second one belongs to $\mathcal{K}_{n+1}^{(0)}$ because adding a zero row/column preserves the cone $\mathcal{K}^{(0)}$. Since adding an isolated node preserves the ϑ -rank 0 property, the next result follows as a direct application of Proposition 4.3.

Lemma 4.7 ([5]). *If ϑ -rank($G \setminus i^\perp$) = 0 for all $i \in V$ then ϑ -rank(G) \leq 1.*

Example 4.8. *As an application of Lemma 4.7 we obtain that ϑ -rank(C_{2n+1}) \leq 1 and ϑ -rank($\overline{C_{2n+1}}$) \leq 1. Moreover, if G is a graph with $\alpha(G) = 2$ then, for all nodes $i \in V$, the graph $G \setminus i^\perp$ is a clique and thus has ϑ -rank 0. Hence, by Lemma 4.7, ϑ -rank(G) \leq 1 and thus Conjecture 1.1 holds for graphs with $\alpha(G) = 2$ (as shown in [5]).*

Let $G = C_5 \oplus i_0$ be the graph obtained by adding one isolated node to the 5-cycle. As shown in [5] G has ϑ -rank 1 and the graph $G \setminus i_0^\perp$ is the 5-cycle which also has ϑ -rank 1. This shows that Lemma 4.7 does not permit to characterize, in general, graphs with ϑ -rank 1. For details on the impact of adding isolated nodes to C_5 see Corollary 6.14.

4.2 Role of critical edges

We finish this section with two results that are useful for bounding the ϑ -rank and show the role of critical edges in this context. On the one hand, deleting non-critical edges can only increase the ϑ -rank. On the other hand, we can strengthen a result from [12] for the class of acritical graphs.

Lemma 4.9 ([19]). *Let $G = (V, E)$ be a graph and let $e \in E$. If e is not a critical edge, i.e., $\alpha(G) = \alpha(G \setminus e)$, then ϑ -rank(G) \leq ϑ -rank($G \setminus e$). Hence, it suffices to show Conjectures 1.1 and 1.2 for the class of critical graphs.*

Remark 4.10. *Let $G = (V, E)$ be a graph. Then one can find a subgraph $H = (V, F)$ of G (with $F \subseteq E$), which is critical and has the same stability number: $\alpha(G) = \alpha(H)$. Indeed to get such a graph H it suffices to delete successively any non-critical edge until getting a subgraph where all edges are critical. Then, by Lemma 4.9, for any such H we have*

$$\vartheta$$
-rank(G) \leq ϑ -rank(H). (4.2)

In the above lemma it was observed that critical edges play a role in the study of the ϑ -rank, namely it would suffice to bound the ϑ -rank of critical graphs. On the other hand, we now prove a stronger version of Conjecture 1.1 for acritical graphs with $\alpha(G) \leq 8$. In [12] the authors proposed the following conjecture and proved that it implies Conjecture 1.1.

Conjecture 4.11 ([12]). *For any $r \geq 1$, we have*

$$\vartheta^{(r)}(G) \leq r + \max_{S \subseteq V, S \text{ stable}, |S|=r} \vartheta^{(0)}(G \setminus S^\perp). \quad (4.3)$$

Theorem 4.12 ([12]). *Conjecture 4.11 holds for $r \leq \min(6, \alpha(G) - 1)$ and for $r = 7 = \alpha(G) - 1$. In particular, Conjecture 1.1 holds for graphs with $\alpha(G) \leq 8$.*

In the case of acritical graphs we can show a stronger bound on the ϑ -rank for graphs with $\alpha(G) \leq 8$.

Proposition 4.13. *Let G be an acritical graph with $\alpha(G) \leq 8$. Then ϑ -rank(G) \leq $\alpha(G) - 2$.*

Proof. It suffices to show that $\vartheta^{(0)}(G \setminus S^\perp) \leq 2$ if S is stable of size $\alpha(G) - 2$ since then the result follows from Eq. (4.3). Let $S = \{i_1, i_2, \dots, i_{\alpha(G)-2}\}$ be a stable set of size $\alpha(G) - 2$ in G , so that $\alpha(G \setminus S^\perp) \leq 2$. If $\alpha(G \setminus S^\perp) = 1$ then $\vartheta^{(0)}(G \setminus S^\perp) = 1$ and we are done. So assume that $\alpha(G \setminus S^\perp) = 2$. Then the graph $H := (G \setminus S^\perp) \oplus S$ is an induced subgraph of G with $\alpha(H) = \alpha(G)$. We claim that H is acritical. This follows from the fact that any critical edge of H should also be a critical edge of G . Indeed, if e is critical in H then there exists a stable set in $H \setminus e$ of size $\alpha(H) + 1 = \alpha(G) + 1$, which is then also stable in $G \setminus e$ as H is an induced subgraph of G , so that e is critical in G . As H is acritical also the graph $G \setminus S^\perp$ is acritical. We claim that $G \setminus S^\perp$ is perfect. For if not then, by the strong perfect graph theorem ([3]), $G \setminus S^\perp$ contains C_5 or $\overline{C_{2n+1}}$ ($n \geq 2$) as an induced subgraph. Since these graphs have stability number equal to $\alpha(G \setminus S^\perp) = 2$ they must be acritical graphs by the above argument. Thus we reach a contradiction since C_5 and $\overline{C_{2n+1}}$ have critical edges. Hence $G \setminus S^\perp$ is perfect and thus we have $\vartheta^{(0)}(G \setminus S^\perp) = \alpha(G \setminus S^\perp) = 2$, which completes the proof. \square

5 Towards characterizing graphs with ϑ -rank 0

In this section we investigate the graphs G with ϑ -rank 0, i.e., such that $\vartheta^{(0)}(G) = \alpha(G)$ or, equivalently, $M_G \in \mathcal{K}_n^{(0)}$. Recall the well-known ‘sandwich inequality’ from [21]:

$$\alpha(G) \leq \vartheta'(G) = \vartheta^{(0)}(G) \leq \vartheta(G) \leq \overline{\chi}(G). \quad (5.1)$$

In view of (5.1), if G can be covered by $\alpha(G)$ cliques then G has ϑ -rank 0. In addition, if $\alpha(G) = \alpha$ and $V_1, V_2, \dots, V_\alpha$ are cliques partitioning V then the matrix

$$P := \begin{pmatrix} (\alpha-1)J & -J & \cdots & -J \\ -J & (\alpha-1)J & \cdots & -J \\ \vdots & \vdots & \ddots & \vdots \\ -J & -J & \cdots & (\alpha-1)J \end{pmatrix},$$

whose block-structure is induced by the partition $V = V_1 \cup \dots \cup V_\alpha$, is a $\mathcal{K}^{(0)}$ -certificate for M_G . In this section we show that the reverse is true for critical graphs and for graphs with $\alpha(G) \leq 2$. We also provide an algorithmic method that permits to reduce the characterization of ϑ -rank 0 graphs to the same property for the class of acritical graphs.

Throughout we often set $\alpha := \alpha(G)$ to simplify notation and we say that a set $S \subseteq V$ is an α -stable set if it is a stable set of size $\alpha(G)$.

5.1 Characterizing critical graphs with ϑ -rank 0

The following result will be repeatedly used.

Lemma 5.1. *Let G be a graph with $\alpha(G) = \alpha$ and let S be an α -stable set. Assume $M_G \in \mathcal{K}_n^{(0)}$ and let P be a $\mathcal{K}^{(0)}$ -certificate for M_G . Then, $\chi^S \in \ker(P)$ and $P[S] = \alpha I_\alpha - J_\alpha$.*

Proof. Directly from Lemma 2.4 since $(\chi^S)^T M_G \chi^S = 0$ as $\chi^S/|S|$ is a global minimizer of (2.8) (recall (2.9)). \square

Proposition 5.2. *Let $G = (V, E)$ be a graph, let E_c denote the set of critical edges of G and let $G_c = (V, E_c)$ be the corresponding subgraph of G . If ϑ -rank(G) = 0 then each connected component of the graph G_c is a clique of G .*

Proof. By assumption, ϑ -rank(G) = 0. Let P be a $\mathcal{K}^{(0)}$ -certificate for M_G . Let V_1, V_2, \dots, V_p be the connected components of the graph G_c . We show that each component V_i is a clique in G . For this pick two nodes $u \neq v \in V_i$ that are connected in G_c . As the edge $\{u, v\}$ is critical, there exists a set $I \subseteq V$ such that $I \cup \{u\}$ and $I \cup \{v\}$ are α -stable in G . Then, by Lemma 5.1, the characteristic vectors $\chi^{I \cup \{u\}}$ and $\chi^{I \cup \{v\}}$ both belong to the kernel of P and thus $\chi^{\{u\}} - \chi^{\{v\}} \in \ker P$. From this we deduce that the columns of P indexed by the nodes in V_i are all equal. Combining this with the fact that the diagonal entries of P are equal to $\alpha - 1$ and that P is symmetric we can conclude that, with respect to the partition $V = V_1 \cup \dots \cup V_p$, the matrix P has the following block-form:

$$P = \begin{pmatrix} (\alpha-1)J_{|V_1|} & a_{12}J_{|V_1| \times |V_2|} & \cdots & a_{1p}J_{|V_1| \times |V_p|} \\ a_{21}J_{|V_2| \times |V_1|} & (\alpha-1)J_{|V_2|} & \cdots & a_{2p}J_{|V_2| \times |V_p|} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1}J_{|V_p| \times |V_1|} & a_{p2}J_{|V_p| \times |V_2|} & \cdots & (\alpha-1)J_{|V_p|} \end{pmatrix} \quad (5.2)$$

for some scalars a_{ij} ($1 \leq i < j \leq p$). We can now show that each V_i is a clique of G . For this pick two distinct nodes $u, v \in V_i$. Then we have $P_{uv} = \alpha - 1 \leq (M_G)_{uv}$, which implies that $(M_G)_{uv} = \alpha - 1$ and thus $\{u, v\}$ is an edge of G . Here we use the fact that the off-diagonal entries of M_G are equal to $\alpha - 1$ for positions corresponding to edges and to -1 for non-edges. Hence we have shown that each component V_i is a clique of G , which concludes the proof. \square

Corollary 5.3. *Assume $G = (V, E)$ is a critical graph, i.e., all its edges are critical. Then we have ϑ -rank(G) = 0 if and only if G is the disjoint union of $\alpha(G)$ cliques. In particular, ϑ -rank(G) = 0 if and only if $\bar{\chi}(G) = \alpha(G)$.*

Proof. The ‘only if’ part follows from Proposition 5.2 and the ‘if part’ follows from Eq. (5.1). The last claim follows directly. \square

Example 5.4. *Let $n \geq 2$. We saw in Remark 4.10 that ϑ -rank(C_{2n+1}) ≤ 1 and ϑ -rank($\overline{C_{2n+1}}$) ≤ 1 . Here we can show, as an application of Corollary 5.3, that their ϑ -rank is equal 1.*

(i) *The graph C_{2n+1} is critical and connected (and not a clique), so by Corollary 5.3, ϑ -rank(C_{2n+1}) ≥ 1 .*

(ii) *The critical edges of the graph $G = \overline{C_{2n+1}}$ are those of the form $\{i, i+2\}$ (for $i \in [2n+1]$, indices taken modulo $2n+1$). Hence the subgraph G_c (of critical edges) is connected (and not a clique) and thus ϑ -rank($\overline{C_{2n+1}}$) ≥ 1 .*

Next we give an example of an acritical graph with ϑ -rank 1.

Example 5.5. Consider the graph H_9 from Figure 2. Note that $\alpha(H_9) = 4$ and that C_9 is a critical subgraph of H_9 with the same stability number. Hence, by Remark 4.10, $\vartheta\text{-rank}(H_9) \leq \vartheta\text{-rank}(C_9) = 1$.

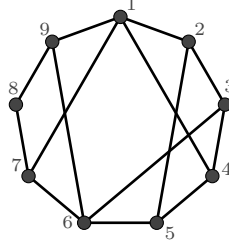


Figure 2: Graph H_9 , acritical

Now, we show that $\vartheta\text{-rank}(H_9) \geq 1$. For this assume, for contradiction, that P is a $\mathcal{K}^{(0)}$ -certificate for M_{H_9} and let C_1, C_2, \dots, C_9 denote the columns of P . Since the sets $\{1, 3, 5, 8\}$, $\{2, 4, 7, 9\}$, $\{3, 5, 7, 9\}$ and $\{2, 4, 6, 8\}$ are stable sets of size 4 in H_9 , by applying Lemma 5.1 we obtain

$$\begin{aligned} (1) \quad C_1 + C_3 + C_5 + C_8 &= 0, & (2) \quad C_2 + C_4 + C_7 + C_9 &= 0, \\ (3) \quad C_3 + C_5 + C_7 + C_9 &= 0, & (4) \quad C_2 + C_4 + C_6 + C_8 &= 0. \end{aligned}$$

By combining (2) and (4) we get that $C_7 + C_9 = C_6 + C_8$. By combining (2) and (3) we get $C_2 + C_4 = C_3 + C_5$. Using these two identities and (2), we get $C_3 + C_5 + C_6 + C_8 = 0$. Finally, using (1) and the last identity we obtain $C_6 = C_1$. This implies $P_{16} = P_{11} = 3 > -1$, which yields a contradiction since $P_{16} \leq -1$ as $\{1, 6\}$ is a non-edge.

5.2 Characterizing graphs with $\alpha(G) = 2$ and $\vartheta\text{-rank}(G) = 0$

Here we observe that the result of Corollary 5.3 holds for all (not necessarily critical) graphs with $\alpha(G) \leq 2$. In Section 5.4 we will show that this also holds for acritical graphs with $\alpha(G) \geq |V| - 4$ (see Proposition 5.17).

Lemma 5.6. Let G be a graph with $\alpha(G) \leq 2$. Then, $\vartheta\text{-rank}(G) = 0$ if and only if $\overline{\chi}(G) = \alpha(G)$.

Proof. It suffices to show the ‘only if’ part. The case $\alpha(G) = 1$ is trivial. So assume $\alpha(G) = 2$ and $\vartheta\text{-rank}(G) = 0$. We show that G is perfect. For if not then, by the strong perfect graph theorem, G contains C_5 or $\overline{C_{2n+1}}$ ($n \geq 2$) as an induced subgraph. Both of these graphs have $\vartheta\text{-rank} 1$ (see Example 5.4). This contradicts Lemma 4.1 which claims that for every induced subgraph H with $\alpha(H) = \alpha(G)$ we must have $\vartheta\text{-rank}(H) \leq \vartheta\text{-rank}(G)$. \square

Example 5.7. We give some examples showing that the characterization in Corollary 5.3 and Lemma 5.6 of rank 0 graphs as those with $\overline{\chi}(G) = \alpha(G)$ does not hold if $\alpha(G) \geq 3$ and G has some non-critical edges.

Let G be the Petersen graph. Then G has rank 0, since $\vartheta(G) = \vartheta^{(0)}(G) = \alpha(G) (= 4)$, but $\overline{\chi}(G) = 5 > \alpha(G) = 4$ (see [21]). Note that the Petersen graph is in fact acritical. The graph $G = \overline{G_{13}}$ considered in [22] provides another example with $3 = \alpha(G) = \vartheta(G) < \overline{\chi}(G) = 4$ and $\vartheta\text{-rank}(G) = 0$.

A class of counterexamples is provided by the Kneser graphs $G_{n,k}$ when $n \geq 2k + 1$ and k does not divide n . Recall $G_{n,k}$ has as vertex set the collection of all k -subsets of $[n]$, where two vertices are adjacent if the corresponding subsets are disjoint. Note that $G_{5,2}$ is the Petersen graph. It has been shown by Lovász [21, 20] that

$$\vartheta(G_{n,k}) = \alpha(G_{n,k}) = \binom{n-1}{k-1} \quad \text{and} \quad \omega(G_{n,k}) (= \alpha(\overline{G_{n,k}})) = \lfloor \frac{n}{k} \rfloor.$$

Therefore $\vartheta\text{-rank}(G_{n,k}) = 0$. However, $\overline{\chi}(G_{n,k}) \geq \binom{n}{k} / \lfloor n/k \rfloor > \binom{n-1}{k-1} = \alpha(G_{n,k})$ if k does not divide n .

Note that $G_{n,k}$ is acritical for any $n > 2k$. To see this one can use a result of Erdős et al. [9] who proved that for $n > 2k$ the maximum stable sets of the Kneser graph $G_{n,k}$ are of the form $\mathcal{A}_j := \{S \subseteq [n] : j \in S, |S| = k\}$ for $j \in [n]$. To see that $G_{n,k}$ is acritical assume for contradiction that $\{A, B\}$ is a critical edge. Then there exists a collection \mathcal{I} of k -subsets of $[n]$ such that $\mathcal{I} \cup \{A\} = \mathcal{A}_i$ and $\mathcal{I} \cup \{B\} = \mathcal{A}_j$ for $i \neq j \in [n]$. Hence, every element of \mathcal{I} contains both i and j , so that $|\mathcal{I}| \leq \binom{n-2}{k-2}$. This gives a contradiction as $|\mathcal{I}| + 1 = |\mathcal{A}_j| = \binom{n-1}{k-1}$.

5.3 Reduction of ϑ -rank 0 graphs to the class of acritical graphs

Here we further investigate the structure of graphs with ϑ -rank 0. We introduce a reduction procedure, which we use to reduce the task of checking the ϑ -rank 0 property to the same property for the class of acritical graphs. This procedure relies on the following graph construction, which is motivated by Lemma 5.2.

Definition 5.8. Let $G = (V, E)$ be a graph and let $G_c = (V, E_c)$ be the subgraph of G , where E_c is the set of critical edges of G . Let V_1, \dots, V_p denote the connected components of G_c . Assume that each of V_1, \dots, V_p is a clique in G . We define the graph $\Gamma(G)$ with vertex set $\{1, 2, \dots, p\}$, where a pair $\{i, j\} \subseteq [p]$ is an edge of $\Gamma(G)$ if $V_i \cup V_j$ is a clique of G .

We show that this graph construction preserves the ϑ -rank 0 property and the stability number.

Lemma 5.9. Assume G is a graph with $\vartheta\text{-rank}(G) = 0$ and let $\Gamma(G)$ be the graph as in Definition 5.8. Then we have: $\vartheta\text{-rank}(\Gamma(G)) = 0$ and $\alpha(\Gamma(G)) = \alpha(G)$.

Proof. Set $\alpha = \alpha(G)$. First, we prove that $\alpha(\Gamma(G)) \geq \alpha$. For this let S be an α -stable set in G and, for each $v \in S$, let V_v denote the connected component of G_c that contains v . Since each V_i is a clique of G (by Lemma 5.2), we have $V_v \neq V_u$ for $u \neq v \in S$ and moreover $V_u \cup V_v$ is not a clique in G . Hence, by definition of the graph $\Gamma(G)$, it follows that the set $\{V_v : v \in S\}$ provides a stable set of size α in $\Gamma(G)$.

Next we show that $\vartheta\text{-rank}(\Gamma(G)) = 0$. By assumption, $\vartheta\text{-rank}(G) = 0$ and thus $M_G = P + N$, where $P \succeq 0$, $N \geq 0$ and $P_{ii} = \alpha - 1$ for all $i \in V$. As shown in the proof of Lemma 5.2, the matrix P has the block-form (5.2) with respect to the partition $V = V_1 \cup \dots \cup V_p$. Then the following $p \times p$ matrix

$$P' := \begin{pmatrix} \alpha - 1 & a_{12} & \cdots & a_{1p} \\ a_{21} & \alpha - 1 & \cdots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \cdots & \alpha - 1 \end{pmatrix}$$

is positive semidefinite. We show that $P' \leq M_{\Gamma(G)}$, thus proving that $\Gamma(G)$ has ϑ -rank 0. As $P' \succeq 0$, we have $|a_{ij}| \leq \alpha - 1 \leq \alpha(\Gamma(G)) - 1$ for all $i, j \in [p]$. It suffices to check that $a_{ij} \leq -1$ if $\{i, j\}$ is not an edge of $\Gamma(G)$. Indeed, in this case, $V_i \cup V_j$ is not a clique in G and thus there exist vertices $u \in V_i$ and $v \in V_j$ such that $\{u, v\}$ is not an edge in G , which implies $a_{ij} = P_{uv} \leq (M_G)_{uv} = -1$. This concludes the proof.

Finally, we prove $\alpha(\Gamma(G)) \leq \alpha$. For this let $I \subseteq [p]$ be an $\alpha(\Gamma(G))$ -stable set. For any $i \neq j \in I$ the set $V_i \cup V_j$ is not a clique in G and thus $a_{ij} \leq -1$ (as observed above). Consider the principal submatrix $P'[I]$ of P' indexed by I . Then we have

$$0 \leq e^T P'[I] e \leq (\alpha - 1)|I| - |I|(|I| - 1),$$

which implies $|I| \leq \alpha$ and thus $\alpha(\Gamma(G)) \leq \alpha$, concluding the proof. \square

Lemma 5.10. Assume $\vartheta\text{-rank}(G) = 0$. Then we have $\bar{\chi}(\Gamma(G)) \geq \bar{\chi}(G)$. In particular, if $\Gamma(G)$ is covered by $\alpha(\Gamma(G))$ cliques, then G is covered by $\alpha(G)$ cliques.

Proof. If $C \subseteq [p]$ is a clique of $\Gamma(G)$, then $\bigcup_{i \in C} C_i$ is a clique in G . Therefore, if we can cover $V(\Gamma(G)) = [p]$ by k cliques of $\Gamma(G)$, then we can cover $V(G)$ by k cliques of G . The last claim follows from the fact that $\alpha(\Gamma(G)) = \alpha(G)$ (Lemma 5.9). \square

Now we provide a partial converse to the result of Lemma 5.9.

Lemma 5.11. Let $G = (V, E)$ be a graph and let $G_c = (V, E_c)$ be its subgraph of critical edges. Assume that the connected components V_1, \dots, V_p of G_c are cliques in G and let $\Gamma(G)$ be as in Definition 5.8. If $\vartheta\text{-rank}(\Gamma(G)) = 0$ and $\alpha(\Gamma(G)) \leq \alpha(G)$, then we have $\vartheta\text{-rank}(G) = 0$.

Proof. By assumption, $\vartheta\text{-rank}(\Gamma(G)) = 0$. Hence there exists a matrix $P \succeq 0$ such that $M_{\Gamma(G)} \geq P$ and $P_{ii} = \alpha_\Gamma := \alpha(\Gamma(G))$ for each $i \in [p]$. Write P as

$$P = \begin{pmatrix} \alpha_\Gamma - 1 & a_{1,2} & \cdots & a_{1,p} \\ a_{2,1} & \alpha_\Gamma - 1 & \cdots & a_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p,1} & a_{p,2} & \cdots & \alpha_\Gamma - 1 \end{pmatrix}$$

and consider the matrix indexed by $V(G) = V_1 \cup \dots \cup V_p$ with the following block-form

$$P' = \begin{pmatrix} (\alpha_\Gamma - 1)J_{|V_1|} & a_{12}J_{|V_1| \times |V_2|} & \cdots & a_{1p}J_{|V_1| \times |V_p|} \\ a_{21}J_{|V_2| \times |V_1|} & (\alpha_\Gamma - 1)J_{|V_2|} & \cdots & a_{2p}J_{|V_2| \times |V_p|} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1}J_{|V_p| \times |V_1|} & a_{p2}J_{|V_p| \times |V_2|} & \cdots & (\alpha_\Gamma - 1)J_{|V_p|} \end{pmatrix}.$$

Then, $P' \succeq 0$. We claim that $P' \leq M_G$ holds. This is true for the diagonal entries and for the positions corresponding to edges of G (since we assume $\alpha_\Gamma \leq \alpha(G)$). Consider now a pair $\{u, v\} \subseteq V$ of vertices that are not adjacent in G . Say $u \in V_i, v \in V_j$. Then, as $V_i \cup V_j$ is not a clique in G , the two vertices $i \neq j \in [p]$ are not adjacent in $\Gamma(G)$ and thus $a_{ij} \leq -1$ since $P \leq M_{\Gamma(G)}$. \square

So we have shown that if we apply the Γ -operator to a graph G with ϑ -rank 0, then we obtain a new graph $\Gamma(G)$ with ϑ -rank 0, with the same stability number and with $|V(\Gamma(G))| \leq |V(G)|$, where the inequality is strict if G has critical edges. We may iterate this construction until obtaining a graph without critical edges.

Definition 5.12. Let G be a graph with ϑ -rank(G) = 0. We define the residual graph $R(G)$ of G as the graph $\Gamma^k(G)$, where k is the smallest integer such that $\Gamma^k(G)$ has no critical edge, after setting $\Gamma^{i+1}(G) = \Gamma(\Gamma^i(G))$ for any $i \geq 0$.

As a direct application of Lemmas 5.9 and 5.10 we obtain the following result.

Lemma 5.13. Let G be a graph with ϑ -rank(G) = 0 and let $R(G)$ be its residual graph as defined in Definition 5.12. Then $R(G)$ has no critical edges and we have ϑ -rank($R(G)$) = 0, $\alpha(R(G)) = \alpha(G)$, and $\bar{\chi}(R(G)) \geq \bar{\chi}(G)$.

Based on the above results, we now present an algorithmic procedure that permits to reduce the task of checking whether a graph has ϑ -rank 0 to the same task restricted to the class of graphs with no critical edges.

Algorithm: REDUCE-TO-ACRITICAL

Input: A graph $G = (V, E)$.

Output: Either: ϑ -rank(G) ≥ 1 . Or: the graph $R(G)$, which is acritical with $\alpha(R(G)) = \alpha(G)$ and such that ϑ -rank(G) = 0 \iff ϑ -rank($R(G)$) = 0.

1. Compute the connected components V_1, V_2, \dots, V_p of the graph $G_c = (V, E_c)$, where E_c is the set of critical edges of G .
2. If V_i is a clique in G for all $i \in [p]$, go to Step 3. Otherwise **return:** ϑ -rank(G) ≥ 1 .
3. Compute the graph $\Gamma(G)$, with set of vertices $\{1, 2, \dots, p\}$ and where $\{i, j\}$ is an edge if $V_i \cup V_j$ is a clique in G . If $\alpha(\Gamma(G)) = \alpha(G)$ then go to Step 4. Otherwise **return:** ϑ -rank(G) ≥ 1 .
4. If $\Gamma(G)$ is acritical then **return:** $\Gamma(G)$. Otherwise set $G = \Gamma(G)$ and go to Step 1.

We verify the correctness of the output of the above algorithm. For this let us assume the algorithm does not output ϑ -rank(G) ≥ 1 . In view of Definition 5.12 the returned graph at step 4 is the residual graph $R(G)$, which is acritical by construction. In addition, in view of Step 3, we have $\alpha(R(G)) = \alpha(G)$. Remains to check that ϑ -rank(G) = 0 if and only if ϑ -rank($R(G)$) = 0. Indeed, the ‘only if’ part follows using iteratively Lemma 5.9, and the ‘if part’ follows using Lemma 5.11.

Observe that, if we apply the above algorithm to a class of graphs with a fixed stability number, then the algorithm runs in polynomial time, so we have shown the following theorem.

Theorem 5.14. For any fixed integer α , the problem of deciding whether a graph with stability number α has ϑ -rank 0 is reducible in polynomial time to the problem of deciding whether a graph with no critical edges and stability number α has ϑ -rank 0.

Example 5.15. We illustrate in Figure 3 the construction of the residual graph $R(G)$ when G is the cycle C_5 with a pendant edge. We show the subgraph G_c (consisting of the critical edges of G) and the graph $\Gamma(G)$, which is critical, so that $\Gamma(G) = \Gamma(G)_c$. Finally, as $\Gamma^2(G) = \overline{K_3}$ has no critical edge, we have $R(G) = \Gamma^2(G) = \overline{K_3}$. Clearly, ϑ -rank($R(G)$) = 0, which shows again ϑ -rank(G) = 0.

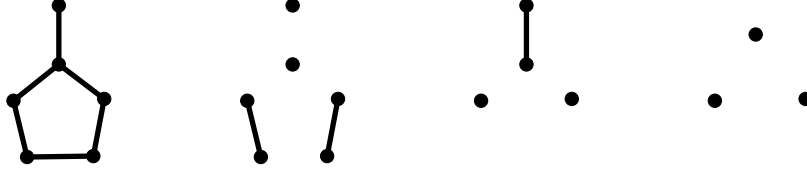


Figure 3: From right to left, the graphs G , G_c (consisting of the critical edges of G), $\Gamma(G)$, $R(G) = \Gamma^2(G)$

Remark 5.16. *The results from this section can be adapted to the Lovász parameter $\vartheta(G)$ instead of $\vartheta^{(0)}(G)$. Recall from [21] that $\vartheta(G) = \alpha(G)$ if and only if there exists a positive semidefinite matrix P such that $P_{ii} = \alpha(G) - 1$ for $i \in V$ and $P_{ij} = -1$ for $\{i, j\} \in E$; call such a P a Lovász-exactness certificate for G . Then one can restate all results from this section by replacing the notion ‘ ϑ -rank(G) = 0’ by ‘ $\vartheta(G) = \alpha(G)$ ’ and the notion of ‘ $\mathcal{K}^{(0)}$ -certificate’ by ‘Lovász-exactness certificate’. As a consequence, we obtain the following analogous result: For any fixed integer α and for graphs with $\alpha(G) = \alpha$, the problem of deciding whether $\vartheta(G) = \alpha$ is reducible in polynomial time to the same problem for graphs with no critical edges.*

5.4 Acritical graphs with large stability number and ϑ -rank 0

Motivated by the reduction to acritical graphs from the previous section, we now consider acritical graphs with large stability number. We show that if $G = (V, E)$ is acritical with $\alpha(G) \geq |V| - 4$, then V can be covered by $\alpha(G)$ cliques and thus G has ϑ -rank 0.

Proposition 5.17. *Let $G = (V, E)$ be a graph and assume $\alpha(G) \geq |V| - 4$.*

- (i) *If $\alpha(G) \geq |V| - 2$ then $\bar{\chi}(G) = \alpha(G)$ and thus ϑ -rank(G) = 0.*
- (ii) *If $\alpha(G) = |V| - 3$ then $\bar{\chi}(G) = \alpha(G)$ and thus ϑ -rank(G) = 0, unless G is the disjoint union of C_5 and isolated nodes in which case ϑ -rank(G) ≥ 1 and G is critical.*
- (iii) *If $\alpha(G) = |V| - 4$ and G is acritical then $\bar{\chi}(G) = \alpha(G)$ and thus ϑ -rank(G) = 0.*

Proof. Throughout we set $\alpha = \alpha(G)$. We will use the fact that perfect graphs satisfy $\chi(\bar{G}) = \alpha(G)$ and their characterization via the strong perfect graph theorem. We distinguish several cases depending on the value of $n = |V|$.

Case 1: $\alpha(G) \geq |V| - 2$.

We claim that G is perfect. For, if not, then G contains an induced subgraph $H = C_{2k+1}$ or $H = \overline{C_{2k+1}}$ ($k \geq 2$); as every stable set of G should exclude at least 3 vertices of H this implies $\alpha(G) \leq |V| - 3$, yielding a contradiction.

Case 2: $\alpha(G) = |V| - 3$.

Let S be an α -stable set and set $V \setminus S = \{x, y, z\}$. Assume G is not covered by α cliques, we show that G is the disjoint union of C_5 and $n - 5$ isolated vertices. As $\bar{\chi}(G) \neq \alpha(G)$ the graph G is not perfect and thus it contains an induced subgraph H which is an odd cycle C_{2k+1} or its complement $\overline{C_{2k+1}}$ with $k \geq 2$. As $|V(H) \cap S| \geq 2k - 2$ it follows that $\alpha(H) \geq 2k - 2$. If $H = C_{2k+1}$ then $\alpha(H) = k \geq 2k - 2$ implies $k \leq 2$ and, if $H = \overline{C_{2k+1}}$, then $\alpha(H) = 2 \geq 2k - 2$ again implies $k \leq 2$. Hence $k = 2$, $H = C_5$, and H contains two nodes of S and the three nodes x, y, z . Say H is the cycle (x, u, y, w, z) with $u, w \in S$. If there exists a node $u_0 \in S \setminus \{u, w\}$ that is adjacent to a node in $\{x, y, z\}$ then one can cover the nodes in $\{u, w, u_0, x, y, z\}$ with three edges and thus V with α cliques, which we had excluded. Therefore, one must have $N_S(\{x, y, z\}) = \{u, w\}$, which implies that G is C_5 together with $n - 5$ isolated nodes.

Case 3: $\alpha(G) = |V| - 4$ and G acritical.

Let S be an α -stable set and set $T = \{x, y, z, w\} = V \setminus S$. Note that every vertex of T has at least two neighbors in S , otherwise the edge between that vertex and S would be a critical edge of G . In addition, if there is a matching between T and S that covers all the nodes in T , then V is covered by α cliques (the four edges of the matching and the remaining $\alpha - 4$ vertices in S) and we are done. Hence we may now assume that there is no matching between S and T that covers T . By Hall’s theorem (see [13]), there exists $W \subseteq T$ such that $|N_S(W)| \leq |W| - 1$. Then $|W| \geq 3$ since $|N_S(W)| \geq 2$. We distinguish two cases.

Case 3a: First assume $|W| = 3$, say $W = \{x, y, z\}$. Then $|N_S(W)| = 2$, say $N_S(W) = \{u, v\}$. So $N_S(x) = N_S(y) = N_S(z) = \{u, v\}$. Since $(S \setminus \{u, v\}) \cup \{x, y, z\}$ is not stable, there is an edge between the vertices x, y, z ,

say $\{x, y\} \in E$. If w has a neighbor in S different from u and v , say $\{w, t\} \in E$ for $t \in S \setminus \{u, v\}$, then V is covered by the cliques $\{x, y, u\}$, $\{z, v\}$, $\{w, t\}$ and the $\alpha - 3$ singleton nodes in $S \setminus \{u, v, t\}$, showing $\bar{\chi}(G) = \alpha(G)$. So we now assume that $N_S(w) = \{u, v\}$. Note that $\bar{\chi}(G) = \alpha(G)$ holds in each of the following two cases: (i) when T contains a clique of size 3 (say, $\{x, y, z\}$) and (ii) when T contains two disjoint edges (say, $\{x, y\}, \{z, w\} \in E$) since then G is covered by the cliques $\{x, y, z, u\}, \{v, w\}$ in case (i), or $\{x, y, u\}, \{z, w, v\}$ in case (ii), and the $\alpha - 2$ singletons in $S \setminus \{u, v\}$. So we may now assume that T does not contain a triangle nor two disjoint edges. But then we reach a contradiction with the fact that each of the two sets $S \setminus \{u, v\} \cup \{x, z, w\}$ and $S \setminus \{u, v\} \cup \{y, z, w\}$ is not a stable set and thus contains an edge.

Case 3b: Assume now $W = T = \{x, y, z, w\}$ and $|N_S(W)| = 2, 3$. If $|N_S(W)| = 2$ then we are in the situation $N_S(x) = N_S(y) = N_S(z) = N_S(w) = \{u, v\} \subseteq S$, already considered in the previous case. So we now assume $|N_S(W)| = 3$, say $N_S(W) = \{u, v, t\} \subseteq S$. We may also assume that G is not perfect (else we are done), so G contains an induced subgraph H which is $\overline{C_{2k+1}}$ with $k \geq 2$. As $V(H) \subseteq W \cup N_S(W)$ we have $2k+1 \leq 7$, so H is C_5, C_7 or $\overline{C_7}$. Note H cannot be $\overline{C_7}$ since $\alpha(\overline{C_7}) = 2$ while the set $\{u, v, t\}$ is stable. If $H = C_7$ then G is C_7 together with $n - 7$ isolated nodes, but then we contradict the assumption that G is acritical. So assume now $H = C_5$. Then $|V(H) \cap S| = 1$ or 2 . We distinguish these two cases:

- Assume $|V(H) \cap S| = 1$, say $V(H) \cap S = \{u\}$ and H is the 5-cycle (x, y, z, w, u) . As H is an induced subgraph of G it follows that $\{y, u\}, \{z, u\} \notin E$. As each of the vertices y and z has at least two neighbors in S , they are both adjacent to both v and t and thus $\{y, z, v\}$ and $\{y, z, t\}$ are cliques. Node w is adjacent to at least two nodes in S and thus w is adjacent to v or t . If w is adjacent to v (resp., to t), then G is covered by the cliques $\{x, u\}, \{y, z, t\}, \{w, v\}$ (resp., $\{y, z, v\}, \{w, t\}$) and the $\alpha - 3$ singletons in $S \setminus \{u, v, t\}$.
- Assume $|V(H) \cap S| = 2$, say $V(H) \cap S = \{u, v\}$ and H is the 5-cycle (x, y, v, z, u) . As x, y must have at least two neighbors in S this implies $\{x, t\}, \{y, t\} \in E$ and thus $\{x, y, t\}$ is a clique. As w has at least two neighbors in S it follows that w is adjacent to u or v . Say, w is adjacent to u . Then G is covered by the cliques $\{x, y, t\}, \{w, u\}, \{z, v\}$ and the $\alpha - 3$ singletons in $S \setminus \{u, v, t\}$. This concludes the proof. \square

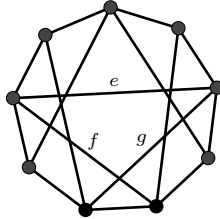


Figure 4: Graph G_9 has $\alpha(G_9) = 4$, $\vartheta(G_9) = \vartheta^{(0)}(G_9) = 4.155$, $\bar{\chi}(G_9) = 5$

- Remark 5.18.** (i) As we just saw in Proposition 5.17 (ii), the only graphs G with $\alpha(G) = |V| - 3$ that do not have ϑ -rank 0 are of the form $G = C_5 \oplus \overline{K_{n-5}}$, the disjoint union of C_5 and $n - 5$ isolated nodes. In fact, we will show that $\vartheta\text{-rank}(C_5 \oplus \overline{K_{n-5}}) = 1$ if and only if $n \leq 13$ (see Corollary 6.14 in Section 6.2).
- (ii) Proposition 5.17 shows that any acritical graph with $\alpha(G) \geq |V| - 4$ satisfies $\bar{\chi}(G) = \alpha(G)$ and thus has ϑ -rank 0. The same holds for graphs with $\alpha(G) = 2$ (Lemma 5.6). The next natural case to consider are graphs with $\alpha(G) = 3$ and $n \geq 8$ nodes. Polak [26] verified (using computer) that if G is an acritical graph on 8 nodes with $\alpha(G) = 3$ then $\bar{\chi}(G) = \alpha(G)$ holds (and thus $\vartheta\text{-rank}(G) = 0$). In addition, if G is acritical on 9 nodes with $\alpha(G) = 3$ then $\vartheta\text{-rank}(G) = 0$ holds as well (but sometimes with $\bar{\chi}(G) > \alpha(G)$). On the other hand there exist acritical graphs on $n = 10$ nodes with $\alpha(G) = 3$ that do not have ϑ -rank 0.
- (iii) There are acritical graphs G with $4 \leq \alpha(G) \leq |V| - 5$ that cannot be covered by $\alpha(G)$ cliques. As a first example consider the graph G_9 in Figure 4, which is acritical, with $|V| = 9$, $\alpha(G_9) = 4$, $\bar{\chi}(G_9) = 5$, and $\vartheta(G_9) = \vartheta^{(0)}(G_9) = 4.155$, and thus $\vartheta\text{-rank}(G_9) \geq 1$. Moreover, with e, f, g being the three labeled edges in G_9 , each of the three graphs $G_9 \setminus e, G_9 \setminus \{f, g\}$ and $G_9 \setminus \{e, f\}$ is acritical and satisfies $\vartheta^{(0)}(G) = \vartheta(G) > \alpha(G)$. This gives four non-isomorphic acritical graphs on 9 vertices that have ϑ -rank at least 1 (and thus cannot be covered by $\alpha(G)$ cliques). Polak [26] verified (using computer) that these are the only non-isomorphic acritical graphs on 9 vertices that do not have ϑ -rank 0.
- (iv) Finally we use the graph H_9 from Example 5.5 to construct a class of acritical graphs with $\bar{\chi}(G) > \alpha(G)$ and $\vartheta\text{-rank}(G) \geq 1$. For any pair (n, α) with $4 \leq \alpha \leq n - 5$, we construct an acritical graph G on n nodes with $\alpha(G) = \alpha$ and $\bar{\chi}(G) > \alpha(G)$. For this we let the vertex set of G be partitioned as $V = V_0 \cup V_1 \cup V_2$, where $|V_0| = 9$, $|V_1| = n - 5 - \alpha$ and $|V_2| = \alpha - 4$, and we select the following edges: on V_0 we put a copy of

H_9 , on V_1 we put a clique, we let every node of V_1 be adjacent to every node of V_0 , and we let V_2 consist of isolated nodes. Then it is easy to see that $\alpha(G) = \alpha$, G is acritical and $\bar{\chi}(G) > \alpha(G)$. One can show that $\vartheta\text{-rank}(G) = \vartheta\text{-rank}(H_9 \oplus \overline{K_{\alpha-4}})$. This follows from the following (easy-to-check) property: If $\{i, j\}$ is an edge and $N(i) \subseteq N(j)$ then $\vartheta\text{-rank}(G \setminus j) = \vartheta\text{-rank}(G)$. Since $\vartheta\text{-rank}(H_9) = 1$ one can now deduce that $\vartheta\text{-rank}(G) \geq 1$.

6 On the impact of isolated nodes on the ϑ -rank

As mentioned in Proposition 4.4, if the ϑ -rank does not increase under the simple graph operation of adding an isolated node then Conjecture 1.1 holds. In [12] it was conjectured that adding isolated nodes indeed does not increase the ϑ -rank. In this section we investigate this question and in fact disprove the latter conjecture, already for graphs with ϑ -rank 1. For this we first observe that critical edges provide a lot of structure on the matrices $P(i)$ ($i \in V$) appearing in $\mathcal{K}^{(1)}$ -certificates, which can be exploited for verifying whether a graph has ϑ -rank 1. Then we investigate the impact of adding isolated nodes to certain classes of graphs H with ϑ -rank 1. First, when the subgraph of critical edges of H is connected, we give an upper bound on the number of isolated nodes that can be added to H while preserving the ϑ -rank 1 property (Theorem 6.6). Second, we show that adding this number of isolated nodes indeed produces a graph with ϑ -rank 1 when H satisfies the property $\vartheta\text{-rank}(H \setminus i^\perp) = 0$ for all its nodes (Theorem 6.13). As an application we are able to determine the exact number of isolated nodes that can be added to an odd cycle C_{2n+1} ($n \geq 2$) or its complement while preserving the ϑ -rank 1 property (see Corollary 6.14). As a byproduct we obtain that adding an isolated node to a graph with ϑ -rank 1 can produce a graph with ϑ -rank ≥ 2 . For instance, $C_5 \oplus \overline{K_8}$ has ϑ -rank 1 but $C_5 \oplus \overline{K_9}$ has ϑ -rank 2.

6.1 Properties of the kernel of $\mathcal{K}^{(1)}$ -certificates

The following results are based on the kernel property observed in Lemma 2.5, which is applied to the matrices M_G and permits to exploit the structure of the graph G .

Lemma 6.1. *Let $G = (V = [n], E)$ be a graph with $\vartheta\text{-rank}(G) = 1$. Let $\{P(i) : i \in V\}$ be a $\mathcal{K}^{(1)}$ -certificate for M_G , let $i \in V$ and let C_1, C_2, \dots, C_n denote the columns of the matrix $P(i)$. Then the following holds.*

- (i) *If S is a stable set of size $\alpha(G)$ and $i \in S$, then we have $\sum_{j \in S} C_j = 0$.*
- (ii) *If $\{i, j\} \in E$ is a critical edge of G then we have $C_i = C_j$.*
- (iii) *If $\alpha(G \setminus i^\perp) = \alpha(G) - 1$ and $\{l, m\} \in E$ is a critical edge of $G \setminus i^\perp$, then we have $C_l = C_m$.*

In particular, if G is critical and $G \setminus i^\perp$ is critical and connected then the matrix $P(i)$ takes the form

$$P(i) = \left(\begin{array}{c|c} (\alpha-1)J_{|i^\perp|} & -1 \\ \hline -1 & \frac{1}{\alpha-1}J_{|V \setminus i^\perp|} \end{array} \right), \quad (6.1)$$

where the blocks are indexed by i^\perp and $V \setminus i^\perp$, respectively.

Proof. Set $\alpha := \alpha(G)$ for short. Part (i) follows directly from Lemma 2.5 (i), which claims $P(i)x = 0$ as $x^T M_G x = 0$ for $x = \chi^S$.

(ii) Since the edge $\{i, j\}$ is critical in G there exists $I \subseteq V$ such that $I \cup \{i\}$ and $I \cup \{j\}$ are α -stable sets in G ; then, using part (i), we get $C_i = -\sum_{k \in I} C_k$. Now, observe that the vector $y = \frac{1}{2\alpha}(\chi^{I \cup \{i\}} + \chi^{I \cup \{j\}})$ satisfies $y^T M y = 0$ (recall Eq. (2.9) and Theorem 2.7). Using Lemma 2.5 (i), we obtain $P(i)y = 0$ and thus $\frac{C_i}{2} + \frac{C_j}{2} + \sum_{k \in I} C_k = 0$. Combining the two equations we get $C_i = C_j$.

(iii) If $\alpha(G \setminus i^\perp) = \alpha - 1$ and $\{l, m\}$ is critical in $G \setminus i^\perp$ then there exists $I \subseteq V$ with $i \in I$ such that $I \cup \{l\}$ and $I \cup \{m\}$ are stable of size α in G . Then, using again part (i), we get $C_l = -\sum_{k \in I} C_k = C_m$.

Finally, assume G is critical and $G \setminus i^\perp$ is critical and connected. Since G is critical, by part (ii), we have $C_i = C_j$ for all $j \in i^\perp$. Moreover, as G is critical, i belongs to an α -stable set and thus $\alpha(G \setminus i^\perp) = \alpha - 1$. Then, part (iii) can be applied and using the connectivity and criticality of $G \setminus i^\perp$ we obtain that $C_l = C_m$ for all $l, m \in V \setminus i^\perp$. Therefore, $P(i)$ takes a block structure indexed by i^\perp and $V \setminus i^\perp$. Using an α -stable set of the form $\{i\} \cup I$ (with $I \subseteq V \setminus i^\perp$) we have $C_i + \sum_{k \in I} C_k = 0$ which, combined with the fact that $P(i)_{ii} = \alpha - 1$, implies the desired structure for the matrix $P(i)$. \square

Using Lemma 6.1 we can show that for some ϑ -rank 1 graphs the construction of the matrices $P(i)$ in a $\mathcal{K}^{(1)}$ -certificate is in fact unique. We already saw that this is the case for the 5-cycle in Example 2.6, we now extend this to any critical graph with $\alpha(G) = 2$ and to the graph $C_5 \oplus i_0$. We show in Figure 5 an example of critical graph with stability number $\alpha(G) = 2$; of course C_5 is another such example.

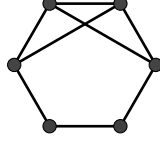


Figure 5: A critical graph with stability number 2

Example 6.2. Let $G = (V, E)$ be a critical graph with $\alpha(G) = 2$. Then $M_G \in \mathcal{K}^{(1)}$ (recall Theorem 4.12). Let $\{P(i) : i \in V\}$ be a $\mathcal{K}^{(1)}$ -certificate for M_G . We show that the matrices $P(i)$ are uniquely determined using Lemma 6.1. Indeed, as $\alpha(G) = 2$, for any $i \in V$ the graph $G \setminus i^\perp$ is a clique and thus it is critical and connected with $\alpha(G \setminus i^\perp) = 1 = \alpha(G) - 1$. Hence Lemma 6.1 can be applied and we obtain that for every $i \in V$ the matrix $P(i)$ takes the form (6.1).

Example 6.3. Let $G = C_5 \oplus i_0 = ([5] \cup \{i_0\}, E)$, so that $G \setminus i_0^\perp = C_5$. As $\alpha(G \setminus i_0^\perp) = \alpha(G) - 1 = 2$ and $G \setminus i_0^\perp$ is critical and connected, by Lemma 6.1 we conclude that the matrix $P(i_0)$ takes the form (6.1) (also displayed below). In particular we have $P(i_0)_{ij} = 1/2$ and $P(i_0)_{i_0i} = -1$ for all $i, j \in [5]$. We now show that for any $i \in [5]$ also the matrices $P(i)$ are uniquely determined; by symmetry it suffices to show this for matrix $P(1)$.

Since G is critical, by Lemma 6.1 (ii) (applied to the edges $\{1, 2\}$ and $\{1, 5\}$), the columns of $P(1)$ indexed by nodes 1, 2, and 5 are identical. As the edge $\{3, 4\}$ is critical in the graph $G \setminus 1^\perp$, by Lemma 6.1 (iii), also the two columns of $P(1)$ indexed by 3 and 4 are identical. This implies that the matrix $P(1)$ takes a block structure indexed by the partition of its index set into $\{1, 2, 5\}$, $\{3, 4\}$ and $\{i_0\}$. By Lemma 2.2 we have $P(1)_{11} = \alpha - 1 = 2$, $2P(1)_{1,i_0} + P(i_0)_{1,1} = \alpha - 3 = 0$ and $P(1)_{i_0,i_0} + 2P(i_0)_{1,i_0} = \alpha - 3 = 0$. Combining with the fact that $P(i_0)_{11} = \frac{1}{2}$ and $P(i_0)_{1,i_0} = -1$ we obtain that $P(1)_{1,i_0} = -\frac{1}{4}$ and $P(1)_{i_0,i_0} = 2$. Finally, since $\{1, 3, i_0\}$ is stable, using Lemma 6.1(i) we obtain that the columns indexed by 1, 3 and i_0 sum up to 0, which enables to complete the rest of the matrix $P(1)$, whose shape is shown below.

$$P(i_0) = \begin{matrix} & i_0 & [5] \\ \begin{matrix} i_0 \\ [5] \end{matrix} & \begin{pmatrix} 2 & -1 \\ -1 & 1/2 \end{pmatrix} \end{matrix}, \quad P(1) = \begin{matrix} & i_0 & \{3, 4\} & \{1, 2, 5\} \\ \begin{matrix} i_0 \\ \{3, 4\} \\ \{1, 2, 5\} \end{matrix} & \begin{pmatrix} 2 & -7/4 & -1/4 \\ -7/4 & 7/2 & -7/4 \\ -1/4 & -7/4 & 2 \end{pmatrix} \end{matrix}.$$

Lemma 6.4. Let $G = (V, E)$ be a graph with $M_G \in \mathcal{K}_n^{(1)}$ and let $P(1), P(2), \dots, P(n)$ be a $\mathcal{K}^{(1)}$ -certificate for M_G . Assume that for $S \subseteq V$ the induced subgraph $G[S]$ is the disjoint union of $\alpha(G)$ cliques.. Then, for any $\{i, j, k\} \subseteq S$, we have

$$P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = (M_G)_{ij} + (M_G)_{jk} + (M_G)_{ik} = \alpha(G) |E(\{i, j, k\})| - 3.$$

Proof. By Theorem 2.7 there exists $x \in \Delta_n$ such that $x^T M_G x = 0$ and $\text{Supp}(x) = S$. Then Lemma 2.5 (ii) gives the desired result. \square

Example 6.5. Consider the graph G_8 shown in Figure 6, which is critical with $\alpha(G_8) = 3$. We show that $\vartheta\text{-rank}(G_8) \geq 2$ (which was verified numerically in [31]). Assume for contradiction that $M_G \in \mathcal{K}_8^{(1)}$ and let $P(1), \dots, P(8)$ be a $\mathcal{K}^{(1)}$ -certificate for M_G . Notice that for $i = 1, 2, 3, 4$ the graph $G \setminus i^\perp = C_5$ is critical and connected. Hence, by Lemma 6.1, the matrices $P(1), P(2), P(3)$ and $P(4)$ take the form (6.1) and thus we have $P(1)_{23} + P(2)_{13} + P(3)_{12} = -1 - 1 + \frac{1}{2} = -\frac{3}{2}$. However, as the graph induced by $\{1, 2, 3, 6\}$ is the disjoint union of $\alpha(G)$ cliques, in view of Lemma 6.4 one should have $P(1)_{23} + P(2)_{13} + P(3)_{12} = 3 \times 1 - 3 = 0$, so we reach a contradiction.

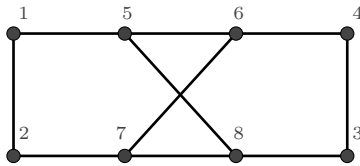


Figure 6: The graph G_8 (critical, $\alpha(G_8) = 3$)

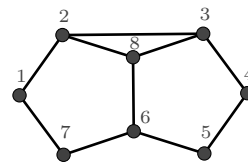


Figure 7: The graph H_8 (critical, $\alpha(H_8) = 3$)

It can also be shown that $\vartheta\text{-rank}(H_8) \geq 2$, the arguments are similar but technical so we omit them. So we have $\vartheta\text{-rank}(G_8) = \vartheta\text{-rank}(H_8) = 2$. In fact, G_8 and H_8 are the only critical graphs on 8 nodes with $\vartheta\text{-rank} = 2$. To see this one can use the list of critical graphs on 8 nodes from [29] and verify that all of them have $\vartheta\text{-rank}$ at most 1 except G_8 and H_8 . Note also that, as observed in [31], any graph with at most 7 nodes has $\vartheta\text{-rank}$ at most 1.

6.2 Adding isolated nodes to graphs with $\vartheta\text{-rank}$ 1

As we saw in Section 4, it is crucial to understand the role of isolated nodes for the $\vartheta\text{-rank}$ of a graph (recall Proposition 4.4). Here we investigate how many isolated nodes can be added to a graph H with $\vartheta\text{-rank}$ 1 (and satisfying certain properties) without increasing its $\vartheta\text{-rank}$. As an application we show that adding an isolated node to some $\vartheta\text{-rank}$ 1 graphs may produce a graph with $\vartheta\text{-rank} \geq 2$.

Throughout this section we consider a graph of the form $G = H \oplus \overline{K_{\alpha-k}}$, where $H = (V, E)$ has $\alpha(H) =: k$, so that $\alpha(G) = \alpha$. Here α and k are integers such that $\alpha \geq k \geq 2$. Note that, if $k = 1$, then H is a clique and thus G has $\vartheta\text{-rank}$ 0 for any α . We let W denote the set of isolated nodes that are added to H , so that $|W| = \alpha - k$ and $G = (V \cup W, E)$. We also consider the subgraph $H_c = (V, E_c)$ of H , where E_c is the set of critical edges of H .

6.2.1 Upper bound on the number of isolated nodes

First, we investigate some necessary conditions about the parameters α and k that must hold if $\vartheta\text{-rank}(G) = 1$.

Theorem 6.6. *Given integers $\alpha > k \geq 2$, let $H = (V, E)$ be a graph with $\alpha(H) = k$ and let $G = H \oplus \overline{K_{\alpha-k}}$. Assume the graph $H_c = (V, E_c)$ is connected and $\vartheta\text{-rank}(G) = 1$. Then we have*

$$\alpha \leq \frac{k(k+3)}{k-1} = k + 4 + \frac{4}{k-1}. \quad (6.2)$$

The rest of the section is devoted to the proof of Theorem 6.6. Throughout we assume that G and H are as defined in Theorem 6.6, so $M_G = \alpha(A_G + I) - J \in \mathcal{K}_n^{(1)}$. We will use the following result of Dobre and Vera [8], which shows the existence of a $\mathcal{K}^{(1)}$ -certificate for M_G , which inherits some symmetry properties of M_G .

Proposition 6.7 ([8]). *Assume that $M \in \mathcal{K}_n^{(1)}$. Then M has a $\mathcal{K}^{(1)}$ -certificate $P(1), \dots, P(n)$ satisfying the following symmetry property: $\sigma(P(i)) = P(\sigma(i))$ for all $\sigma \in \text{Sym}(n)$ such that $\sigma(M) = M$.*

So let $\{P(i) : i \in V\}$ be a $\mathcal{K}^{(1)}$ -certificate for M_G satisfying the symmetry property from Proposition 6.7. In particular, since any permutation $\sigma \in \text{Sym}(W)$ of the isolated nodes leaves the graph G invariant it follows that

$$\sigma(P(i)) = P(\sigma(i)), \text{ i.e., } P(i)_{\sigma(j)\sigma(k)} = P(\sigma(i))_{jk} \text{ for all } \sigma \in \text{Sym}(W) \text{ and } j, k \in V \cup W. \quad (6.3)$$

We will use this symmetry property repeatedly in the proof. We mention a simple identity that follows as a direct application of Lemma 6.4, which we will also repeatedly use in the rest of the section:

$$P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = -3 \quad \text{if } \{i, j, k\} \text{ is contained in a stable set of } G \text{ with size } \alpha(G). \quad (6.4)$$

Now we prove some preliminary lemmas and we end with Lemma 6.11, which will directly imply Theorem 6.6. We start with a general property about the structure of the submatrices $P(i)[W]$ when $i \in W$ is an isolated node.

Lemma 6.8. *There exists a scalar $b \in \mathbb{R}$ such that the following holds:*

- (i) $P(i)_{ij} = b$ for all distinct $i, j \in W$,
- (ii) $P(i)_{jj} = \alpha - 2b - 3$ for all distinct $i, j \in W$,
- (iii) $P(i)_{jk} = -1$ for all distinct $i, j, k \in W$.

Proof. Let $i, j, k \in W$ be distinct (isolated) nodes and set $b := P(i)_{ij}$. First we show that b does not depend on the choice of $i, j \in W$. For this we use the symmetry property from (6.3), which claims $P(i)_{\sigma(i)\sigma(j)} = P(\sigma(i))_{ij}$ for any $\sigma \in \text{Sym}(W)$. Using the permutation $\sigma = (j, k)$ we get $P(i)_{ij} = P(i)_{ik} = b$, and using $\sigma = (i, j)$ we get $P(i)_{ij} = P(j)_{ij} = b$, thus showing (i). Now, by Lemma 2.2, we have $P(i)_{jj} + 2P(j)_{ij} = \alpha - 3$, which implies $P(i)_{jj} = \alpha - 2b - 3$ and thus (ii) holds. Using again (6.3) with $\sigma = (i, k)$ we obtain $P(i)_{\sigma(i)\sigma(j)} = P(\sigma(i))_{i,j}$, and thus $P(i)_{jk} = P(k)_{ij}$. Similarly, using $\sigma = (i, j)$ we get $P(i)_{\sigma(i)\sigma(k)} = P(\sigma(i))_{ik}$ and thus $P(i)_{jk} = P(j)_{ik}$. By using Eq. (6.4) for the nodes i, j, k we obtain $P(i)_{jk} = P(j)_{ik} = P(k)_{ij} = -1$, thus showing (iii). \square

So we know the structure of the submatrix $P(i)[W]$ when $i \in W$ is an isolated node. When the graph H_c (consisting of the critical edges of H) is connected we can also derive the structure of the rest of the matrix $P(i)$.

Lemma 6.9. *Assume the graph H_c is connected. Then the matrix $P(i)$ takes the form*

$$P(i) = \begin{array}{c} i \\ W \setminus i \\ V \end{array} \begin{array}{c} i \\ W \setminus i \\ V \end{array} \begin{array}{c} W \setminus i \\ V \end{array} \begin{array}{c} d \dots d \\ \beta J \\ d \\ \vdots \\ d \end{array} \begin{array}{c} \beta J \\ \gamma J \end{array} \quad \text{for all } i \in W,$$

where the blocks are indexed by $\{i\}$, $W \setminus \{i\}$ and V , respectively, and the scalars d, β, γ are given by

$$d = \frac{b(k+1) + 1 - \alpha - b\alpha}{k}, \quad \beta = \frac{b+1-k}{k}, \quad \gamma = \frac{\alpha-k}{k}.$$

Proof. Fix an isolated node $i \in W$. Let $\{l, m\} \in E_c$ be a critical edge of H . By Lemma 6.1(iii) we get that the two columns of $P(i)$ indexed by l and m are identical. Since H_c is connected it follows that the columns of $P(i)$ indexed by V are all identical. From this follows that $P(i)[V]$ (the submatrix of $P(i)$ indexed by V) is of the form $\gamma_i J$ for some scalar γ_i and there exists a vector $b_i \in \mathbb{R}^W$ such that $P(i)_{jh} = (b_i)_j$ for all $j \in W, h \in V$.

Let $j \neq k \in W \setminus \{i\}$ and $v \in V$. By applying Eq. (6.3) to the permutation $\sigma = (j, k)$, we obtain $P(i)_{\sigma(k)\sigma(v)} = P(\sigma(i))_{kv}$, and thus $P(i)_{jv} = P(i)_{kv}$. Therefore, the entries of b_i indexed by $W \setminus \{i\}$ are all equal, say to a scalar β_i . We set $d_i := (b_i)_i$. Finally we show that the scalars β_i, γ_i, d_i in fact do not depend on the choice of $i \in W$ and take the values claimed in the lemma.

For this consider an α -stable set S of G . Then $i \in S$ and thus, by Lemma 6.1(i), the columns of $P(i)$ indexed by S sum up to zero. Using the identities of Lemma 6.8 combined with the above facts on the remaining entries of $P(i)$, we obtain

$$\begin{aligned} (\alpha - 1) + (\alpha - k - 1)b + kd_i = 0 &\implies d_i = \frac{b(k+1) + 1 - \alpha - b\alpha}{k}, \\ b - (\alpha - k - 2) + (\alpha - 2b - 3) + k\beta_i = 0 &\implies \beta_i = \frac{b+1-k}{k}, \\ d_i + (\alpha - k - 1)\beta_i + k\gamma_i = 0 &\implies \gamma_i = \frac{\alpha-k}{k}. \end{aligned}$$

This concludes the proof. \square

We now are able to conclude some properties on the structure of the matrices $P(j)$ for $j \in V$.

Lemma 6.10. *Assume H_c is connected. For any $v \in V$ the submatrix $P(v)[W \cup \{v\}]$ takes the form*

$$P(v)[W \cup \{v\}] = \left(\begin{array}{c|c} M_b & \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \\ \hline \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & \alpha - 1 \end{array} \right), \quad (6.5)$$

where the blocks are indexed by W and $\{v\}$, respectively. Here, $b \in \mathbb{R}$ is the constant from Lemma 6.8 and the matrix M_b is indexed by V and takes the form

$$M_b = \begin{pmatrix} a & c & \dots & c \\ c & a & \dots & c \\ \vdots & \vdots & \ddots & \vdots \\ c & c & \dots & a \end{pmatrix}, \quad \text{with } a = \alpha - 3 - \frac{2}{k}(b(k+1) + 1 - \alpha - b\alpha), \quad c = -1 - \frac{2}{k}(b+1). \quad (6.6)$$

Proof. Consider an isolated node $i \in W$. By Lemma 2.2 we have $P(v)_{ii} + 2P(i)_{iv} = \alpha - 3$. This implies $P(v)_{ii} = \alpha - 3 - 2d$ and thus $P(v)_{ii} = \alpha - 3 - \frac{2}{k}(b(k+1) + 1 - \alpha - b\alpha)$, which shows the claimed value of a .

Consider $i \neq j \in W$. As H_c is connected, v belongs to a critical edge and thus there exists an α -stable set of G that contains i, j, v . Then, by (6.4), we have $P(i)_{vj} + P(j)_{iv} + P(v)_{ij} = -3$. This implies $P(v)_{ij} = -3 - 2\beta$ and thus $P(v)_{ij} = -1 - \frac{2(b+1)}{k}$, which shows the claimed value of c .

Let $i \in W$. Using again Lemma 2.2 we get $2P(v)_{iv} + P(i)_{vv} = \alpha - 3$. Hence $P(v)_{iv} = \frac{\alpha-3-\gamma}{2}$, which implies $P(v)_{iv} = \frac{\alpha}{2} - \frac{\alpha}{2k} - 1$. This completes the proof. \square

The following lemma gives necessary and sufficient conditions for the matrix in Eq. (6.5) to be positive semidefinite. In particular, the part (ii) of the lemma shows Theorem 6.6.

Lemma 6.11. *The matrix in Eq. (6.5) is positive semidefinite if and only if the following two conditions hold:*

- (i) $a \geq c$,
- (ii) $\alpha \leq k + 4 + \frac{4}{k-1}$.

Proof. By taking the Schur complement of the matrix $P(v)[W \cup \{v\}]$ in (6.5) with respect to its (v, v) -entry we obtain that $P(v)[W \cup \{v\}] \succeq 0$ if and only if

$$(a - c)I_{\alpha-k} + \left(c - \frac{1}{\alpha-1} \left(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1\right)^2\right) J_{\alpha-k} \succeq 0.$$

This happens if and only $a \geq c$ and the following inequality holds:

$$a - c + (\alpha - k) \left(c - \frac{1}{\alpha-1} \left(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1\right)^2\right) \geq 0.$$

We show that this last inequality holds if and only if (ii) holds. First, notice that $a + (\alpha - k - 1)c = k$. Indeed, if we see this expression as a polynomial in b then the coefficient of b is

$$-\frac{2}{k}(k - \alpha + 1) - \frac{2}{k}(\alpha - k - 1) = 0$$

and the constant coefficient is

$$\alpha - 3 - \frac{2(1 - \alpha)}{k} + (\alpha - k - 1)\left(-1 - \frac{2}{k}\right) = k.$$

Therefore, the inequality $a - c + (\alpha - k)\left(c - \frac{1}{\alpha-1} \left(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1\right)^2\right) \geq 0$ is equivalent to

$$k(\alpha - 1) \geq (\alpha - k) \left(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1\right)^2.$$

Multiplying both sides by $4k^2$, this is equivalent to

$$\begin{aligned} 4k^3(\alpha - 1) &\geq (\alpha - k)(\alpha(k - 1) - 2k)^2 \\ \iff 4k^3\alpha - 4k^3 &\geq (\alpha - k)(\alpha^2(k - 1)^2 - 4k(k - 1)\alpha + 4k^2) \\ \iff 4k^3\alpha - 4k^3 &\geq \alpha^3(k - 1)^2 - \alpha^2k(k - 1)^2 - 4\alpha^2k(k - 1) + 4\alpha k^3 - 4k^3 \end{aligned}$$

after cancelling terms in the right hand side. Cancelling terms at both sides and dividing by $\alpha^2(k - 1)$ (as $k \geq 2$) we obtain $\alpha(k - 1) - 4k - k(k - 1) \leq 0$ and thus the desired inequality (ii). \square

6.2.2 Lower bound on the number of isolated nodes

In Theorem 6.6 we saw that if the subgraph H_c of critical edges of H is connected and the graph $G = H \oplus \overline{K_{\alpha-k}}$, obtained by adding $\alpha - k$ isolated nodes to a graph H with $\alpha(H) = k$, has ϑ -rank 1, then the parameters α and k must satisfy the inequality (6.2). So this gives the upper bound $\alpha - k \leq 4 + 4/(k - 1)$ on the number of isolated nodes that can be added while preserving the ϑ -rank 1 property.

Here we provide some classes of graphs H for which it is indeed possible to add this maximum number of isolated nodes and preserve the ϑ -rank 1 property. Hence, for these graphs, we characterize the exact number of isolated nodes that can be added while preserving the ϑ -rank 1 property.

We begin with a preliminary lemma which we will use for our main result below.

Lemma 6.12. *Assume $\alpha \geq k \geq 2$ satisfy the inequality (6.2), and let $M := \alpha I_{\alpha-k} - J_{\alpha-k}$. Then*

$$\left(\frac{M}{\frac{\alpha}{2} - \frac{\alpha}{2k} - 1} \mid \frac{\frac{\alpha}{2} - \frac{\alpha}{2k} - 1}{\alpha - 1}\right) \succeq 0.$$

Proof. The above matrix corresponds to the matrix in Eq. (6.5) with $b = -1$, which gives $a = \alpha - 1$ and $c = -1$, so that $M = M_b = M_{-1}$. As $a \geq c$, using Lemma 6.11, we get the desired result. \square

Theorem 6.13. *Given integers $\alpha \geq k \geq 2$, let $H = (V, E)$ be a graph with $\alpha(H) = k$ and let $G = H \oplus \overline{K_{\alpha-k}}$. Assume that $\vartheta\text{-rank}(H \setminus i^\perp) = 0$ for all $i \in V$ and $\vartheta\text{-rank}(H) = 1$. In addition assume that α, k satisfy the inequality (6.2). Then we have $\vartheta\text{-rank}(G) = 1$.*

Proof. We construct a $\mathcal{K}^{(1)}$ -certificate for the matrix M_G . That is, we construct matrices $P(i)$ (for $i \in W \cup V$) that satisfy the properties of Lemma 2.2. Recall Remark 2.3 where we observed that it will suffice to show that the matrices $P(i)$ belong to the cone $\mathcal{K}^{(0)}$. For this consider the following construction (inspired from [12]), where we set $M := \alpha I_{\alpha-k} - J_{\alpha-k}$.

• For $i \in V$, we set

$$P(i) = \left(\begin{array}{c|c|c} M & \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & -\frac{\alpha}{2k} - 1 \\ \hline \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & \alpha - 1 & \frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} \\ \hline -\frac{\alpha}{2k} - 1 & \frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} & \begin{cases} \frac{\alpha^2}{k} - 1 & \text{if } i \simeq j \\ -1 & \text{else} \end{cases} \end{array} \right),$$

where the blocks are indexed by W , i^\perp and $V \setminus i^\perp$, respectively. Here the notation $i \simeq j$ means that the nodes i and j are equal or adjacent in G .

• For $i \in W$, we set

$$P(i) = \left(\begin{array}{c|c} M & -1 \\ \hline -1 & \frac{\alpha-k}{k} J \end{array} \right),$$

where the blocks are indexed by W and V , respectively.

First we show that the matrix $P(i)$ is positive semidefinite for all $i \in W$. Indeed, deleting repeated rows and columns and taking the Schur complement with respect to the lower right corner we obtain that $P(i) \succeq 0$ if and only if $0 \leq M - \frac{k}{\alpha-k} J_{\alpha-k} = \alpha I_{\alpha-k} - \frac{\alpha}{\alpha-k} J_{\alpha-k}$, which is indeed true.

Next we show that $P(i) \in \mathcal{K}^{(0)}$ for all $i \in V$. For this, let $i \in V$ and observe that we can decompose $P(i)$ as $P(i) = Q(i) + \frac{\alpha^2}{k(k-1)} R(i)$, where

$$Q(i) = \left(\begin{array}{c|c|c} M & \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & -\frac{\alpha}{2k} - 1 \\ \hline \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & \alpha - 1 & \frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} \\ \hline -\frac{\alpha}{2k} - 1 & \frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} & \frac{\alpha^2}{k(k-1)} - 1 \end{array} \right) \text{ and } R(i) = \left(\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & 0 & 0 \\ \hline 0 & 0 & \begin{cases} k-2 & \text{if } i \simeq j \\ -1 & \text{else} \end{cases} \end{array} \right),$$

whose blocks are indexed by W , i^\perp and $V \setminus i^\perp$, respectively. We prove that $Q(i) \succeq 0$ and $R(i) \in \mathcal{K}^{(0)}$.

First, we show that $Q(i)$ is positive semidefinite. By Lemma 6.12 we know that the submatrix $Q(i)[W \cup i^\perp]$ is positive semidefinite. We will now show that any column C_v of $Q(i)$ indexed by a node $v \in V \setminus i^\perp$ (in the third block) can be expressed as a linear combination of the columns C_u indexed by $u \in W \cup \{i\}$ (in the first two blocks), which directly implies that $Q(i) \succeq 0$. Namely, one can show $C_v = \frac{1}{1-k} (\sum_{j \in W} C_j + C_i) =: C$ by direct inspection of the entries:

- for the entries indexed by $u \in I$ we have:

$$C_u = \frac{1}{1-k} \left(\alpha - 1 - (\alpha - k - 1) + \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \right) = -1 - \frac{\alpha}{2k} = (C_v)_u,$$

- for the entries indexed by $u \in i^\perp$ we have:

$$C_u = \frac{1}{1-k} \left((\alpha - k) \left(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \right) + \alpha - 1 \right) = -1 + \frac{\alpha}{2} - \frac{\alpha^2}{2k},$$

- for the entries indexed by $u \in V \setminus i^\perp$ we have:

$$C_u = \frac{1}{1-k} \left((\alpha - k) \left(-\frac{\alpha}{2k} - 1 \right) + \frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} \right) = \frac{\alpha^2}{k(k-1)} - 1.$$

Now we show that $R(i) \in \mathcal{K}^{(0)}$. For this note that $\alpha(H \setminus i^\perp) \leq k - 1$, which implies the entry-wise inequality

$$\left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & M_{H \setminus i^\perp} \end{array} \right) \leq R(i).$$

By hypothesis $M_{H \setminus i^\perp} \in \mathcal{K}^{(0)}$. Since adding zero row/columns preserve membership in $\mathcal{K}^{(0)}$ we get that $R(i) \in \mathcal{K}^{(0)}$.

To conclude the proof we now need to check that the linear constraints (ii)-(iv) of Lemma 2.2 are satisfied by the matrices $P(i)$. This is direct case checking, but we give the details for clarity.

Identity (ii): $P(v)_{vv} = \alpha - 1 = (M_G)_{vv}$ for all $v \in V \cup I$.

Identity (iii): We check that $P(u)_{vv} + 2P(v)_{uv} = (M_G)_{vv} + 2(M_G)_{uv}$ for all $u \neq v \in I \cup V$:

- for $i, j \in I$, we have $P(i)_{jj} + 2P(j)_{ij} = \alpha - 1 - 2 = \alpha - 3$,
- for $i \in I, v \in V$, we have
 - $P(i)_{vv} + 2P(v)_{iv} = \frac{\alpha-k}{k} + \alpha - \frac{\alpha}{k} - 2 = \alpha - 3$,
 - $P(v)_{ii} + 2P(i)_{iv} = \alpha - 1 - 2 = \alpha - 3$,
- for $u, v \in V$, we have
 - if $\{u, v\} \in E$ then $P(u)_{vv} + 2P(v)_{uv} = 3\alpha - 3$,
 - if $\{u, v\} \notin E$ then $P(u)_{vv} + 2P(v)_{uv} = \frac{\alpha^2}{k} - 1 + 2(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}) = \alpha - 3$.

Inequality (iv): We check $P(u)_{vw} + P(v)_{uw} + P(w)_{uv} \leq (M_G)_{uv} + (M_G)_{vw} + (M_G)_{vw}$ for distinct $u, v, w \in I \cup V$:

- for $i, j, k \in I$ we have $P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = -3$,
- for $i, j \in I, v \in V$ we have $P(i)_{jv} + P(j)_{iv} + P(v)_{ij} = -3$,
- for $i \in I, u, v \in V$ we have
 - if $\{u, v\} \notin E$ then $P(i)_{uv} + P(u)_{iv} + P(v)_{iu} = \frac{\alpha-k}{k} - 2(\frac{\alpha}{2k} + 1) = -3$,
 - if $\{u, v\} \in E$ then $P(i)_{uv} + P(u)_{iv} + P(v)_{iu} = \frac{\alpha-k}{k} + 2(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1) = \alpha - 3$,
- for $u, v, w \in V$ we have
 - if $\{u, v\}, \{v, w\}, \{u, w\} \in E$ then $P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = 3(\alpha - 1)$,
 - if $\{u, v\}, \{u, w\} \in E, \{v, w\} \notin E$ then $P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = \alpha - 1 + 2(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}) = 2\alpha - 3 - \frac{\alpha^2}{2k} \leq 2\alpha - 3$,
 - if $\{u, v\} \in E, \{u, w\}, \{v, w\} \notin E$ then $P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = 2(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}) + \frac{\alpha^2}{k} - 1 = \alpha - 3$,
 - if $\{u, v\}, \{u, w\}, \{v, w\} \notin E$ then $P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = -3$.

This completes the proof. □

We now give some examples of graphs for which the conditions of Theorem 6.6 and 6.13 hold, so that we are able to compute the exact number of isolated nodes that can be added with the resulting graph still having ϑ -rank 1.

Corollary 6.14. *For any integer $n \geq 2$ the following holds:*

- (i) ϑ -rank($C_{2n+1} \oplus \overline{K_m}$) = 1 if and only if $m \leq 4 + \frac{4}{n-1}$.
- (ii) ϑ -rank($\overline{C_{2n+1}} \oplus \overline{K_m}$) = 1 if and only if $m \leq 8$.

Proof. Consider the graph $H = C_{2n+1}$ or $H = \overline{C_{2n+1}}$. As pointed out in Example 4.8, H satisfies the property: ϑ -rank($H \setminus i^\perp$) = 0 for all $i \in V$, and thus the assumption of Theorem 6.13 holds. For $H = C_{2n+1}$ the inequality (6.2) reads $m \leq 4 + \frac{4}{n-1}$ and, for $H = \overline{C_{2n+1}}$, it reads $m \leq 8$. So the ‘if part’ in both (i), (ii) follows as a direct application of Theorem 6.13.

The ‘only if’ part in both (i), (ii) follows as a direct application of Theorem 6.6, since the graph C_{2n+1} is critical while the subgraph of critical edges of $\overline{C_{2n+1}}$ is a connected graph. □

Corollary 6.15. *Assume H is a graph with $\overline{\chi}(H) > \alpha(H) = 2$. Then, ϑ -rank($H \oplus \overline{K_m}$) = 1 if and only if $m \leq 8$.*

Proof. The ‘if’ part follows directly from Theorem 6.13. Now we prove that ϑ -rank($H \oplus \overline{K_m}$) ≥ 2 for $m \geq 9$. Since H is not perfect it contains the graph $H_0 = C_5$ or $H_0 = \overline{C_{2n+1}}$ ($n \geq 2$) as an induced subgraph. Hence, $H_0 \oplus \overline{K_m}$ is an induced subgraph of $H \oplus \overline{K_m}$ with the same stability number. Then, by Lemma 4.1, ϑ -rank($H \oplus \overline{K_m}$) $\geq \vartheta$ -rank($H_0 \oplus \overline{K_m}$) ≥ 2 , where the last inequality follows from Corollary 6.14. □

Corollary 6.16. *Consider a graph H and a connected component H_0 of H . Assume $\alpha(H_0) \geq 2$ and the subgraph $(H_0)_c$ of critical edges of H_0 is connected. Then the following holds:*

- (i) If $\alpha(H) \geq \alpha(H_0) + 9$ then ϑ -rank(H) ≥ 2 .

(ii) If $\alpha(H) \leq \alpha(H_0) + 8$ then $\vartheta\text{-rank}(H \oplus \overline{K_s}) \geq 2$ for $s \geq 9 - \alpha(H) + \alpha(H_0)$.

Proof. By Corollary 5.3 we know $\vartheta\text{-rank}(H_0) \geq 1$. Pick a stable set $W \subseteq V(H \setminus H_0)$ such that $\alpha(H_0 \oplus W) = \alpha(H)$, i.e., $|W| = \alpha(H) - \alpha(H_0)$. Then $H_0 \oplus W$ is an induced subgraph of H with the same stability number as H . Then, by Lemma 4.1, $\vartheta\text{-rank}(H_0 \oplus W \oplus \overline{K_s}) \leq \vartheta\text{-rank}(H \oplus \overline{K_s})$ for any $s \geq 0$. By applying Corollary 6.15 to the graph H_0 , we obtain that $\vartheta\text{-rank}(H_0 \oplus W \oplus \overline{K_s}) \geq 2$ if $s + |W| \geq 9$. From these facts (i) and (ii) now follow easily. \square

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