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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 introduced in 2002 semidefinite bounds $\vartheta^{(r)}(G)$ ($r \geq 0$) for the stability number $\alpha(G)$ of a graph G and conjectured their exactness at order $r = \alpha(G) - 1$. These bounds rely on the conic approximations $\mathcal{K}_n^{(r)}$ introduced by Parrilo in 2000 for the copositive cone COP_n . A difficulty in the convergence analysis of the bounds is the bad behavior of Parrilo’s cones under adding a zero row/column: when applied to a matrix not in $\mathcal{K}_n^{(r)}$ this gives a matrix that does not lie in any of Parrilo’s cones, thereby showing that their union is a strict subset of the copositive cone for any $n \geq 6$. We investigate the graphs for which the bound of order $r \leq 1$ is exact: we algorithmically reduce testing exactness of $\vartheta^{(0)}$ to acritical graphs, we characterize the 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 posed by Gvozdenović and Laurent in 2007, which, if true, would have implied the above conjecture by de Klerk and Pasechnik.

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

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 Bomze et al. [1], Hossain et al. [15], Wu and Hao [32], and references therein). This problem is well-known to be NP-hard (Karp [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 are introduced in de Klerk and Pasechnik [4] 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 of 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 de Klerk and Pasechnik [4] for the stability number:

$$\alpha(G) = \min\{t : t(I + A_G) - J \in \text{COP}_n\}. \quad (1)$$

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), the following *graph matrix*

$$M_G := \alpha(G)(A_G + I) - J \quad (2)$$

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

$$F_G(x) := (x^{\circ 2})^T M_G x^{\circ 2} \tag{3}$$

is nonnegative on \mathbb{R}^n . A natural question is whether there exist certificates for copositivity of M_G based on semidefinite programming and 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 [25] and defined by

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^T M x^{\circ 2} \in \Sigma \right\} \text{ for } r \in \mathbb{N}, \tag{4}$$

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

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n. \tag{5}$$

Starting from the copositive formulation (1) and using the cones $\mathcal{K}_n^{(r)}$, De Klerk and Pasechnik [4] introduce the following hierarchy of approximations for $\alpha(G)$:

$$\vartheta^{(r)}(G) = \min\{t : t(A_G + I) - J \in \mathcal{K}_n^{(r)}\}, \tag{6}$$

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 (6). As sums of squares of polynomials can be modeled 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 Laurent and Vargas [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 these notions: for any integer $r \in \mathbb{N}$, we have

$$M_G \in \mathcal{K}_n^{(r)} \iff \left(\sum_{i=1}^n x_i^2 \right)^r F_G \in \Sigma \iff \vartheta^{(r)}(G) = \alpha(G) \iff \vartheta\text{-rank}(G) \leq r. \tag{7}$$

de Klerk and Pasechnik [4] conjecture that the hierarchy $\vartheta^{(r)}(G)$ converges to $\alpha(G)$ in at most $\alpha(G) - 1$ steps, which shows that this continuous copositive-based hierarchy has the same convergence behavior as the Lasserre hierarchy based on discrete formulations of $\alpha(G)$ (Lasserre [17], Laurent [18]). In view of (7), this can be reformulated as follows.

Conjecture 1 (de Klerk and Pasechnik [4]). *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 2 (Laurent and Vargas [19]). *For a graph G , any of the following equivalent claims holds: (i) $M_G \in \cup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)}$, (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 Gvozdenović and Laurent [12], Conjecture 1 is shown to hold for all graphs with $\alpha(G) \leq 8$ (see also Peña et al. [26] for the case $\alpha(G) \leq 6$). In Laurent and Vargas [19] it is observed that it suffices to prove both Conjectures 1 and 2 for the class of critical graphs, that is, for the graphs G satisfying $\alpha(G \setminus e) = \alpha(G) + 1$ for all edges e of G . In addition, it is shown in Laurent and Vargas [19] that Conjecture 2 holds for acritical graphs, that is, for the graphs G satisfying $\alpha(G \setminus e) = \alpha(G)$ for all edges.

1.1. Some Possible Directions for Resolving Conjectures 1 and 2

In what follows, we mention some possible strategies that could be followed to attack these 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 Dickinson et al. [7] that any copositive matrix with diagonal entries zero or one 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 2. However, we disprove the conjecture from Dickinson

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et al. [7] for matrix size $n \geq 6$ (see Section 3). In particular, this shows that the inclusion $\cup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$ in (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 3 (Gvozdenović and Laurent [12]). *For any graph G , we have $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G)$.*

Conjecture 4. *For any graph G , $\vartheta\text{-rank}(G) < \infty$ implies $\vartheta\text{-rank}(G \oplus i_0) < \infty$.*

Conjecture 3 is in fact posed in Gvozdenović and Laurent [12] in a more general form (see Gvozdenović and Laurent [12, conjecture 4]). In addition, it is shown in Gvozdenović and Laurent [12] that Conjecture 3 implies Conjecture 1.

We show that Conjecture 4 is, in fact, equivalent to Conjecture 2 (see Proposition 4). 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 Gvozdenović and Laurent [12], in which we set $\alpha := \alpha(G)$ so that $\alpha(G \oplus i_0) = \alpha + 1$:

$$M_{G \oplus i_0} = \begin{pmatrix} \alpha & & -1 \\ & & \\ -1 & (\alpha + 1)(I + A_G) - J & \end{pmatrix} = \begin{pmatrix} \alpha & -1 \\ -1 & \frac{1}{\alpha} J \end{pmatrix} + \frac{\alpha + 1}{\alpha} \begin{pmatrix} 0 & 0 \\ 0 & \alpha(I + A_G) - J \end{pmatrix}. \quad (8)$$

If the operation of adding a zero row/column preserves membership in the cones $\mathcal{K}^{(r)}$ then, in view of (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 3 (and, thus, also Conjecture 1). In addition, if adding a zero row/column preserves membership in the union $\cup_{r \in \mathbb{N}} \mathcal{K}^{(r)}$, then, again in view of (8), Conjecture 4 is true and, thus, Conjecture 2 too. However, adding a zero row/column does *not*, in general, preserve membership in the cones $\mathcal{K}^{(r)}$ for a given order $r \geq 1$ (whereas this is clearly true for order $r = 0$); this is observed (numerically) for order $r = 1$ using the graph matrix $M_{C_5} \in \mathcal{K}_5^{(1)}$ of the five-cycle (see de Klerk and Pasechnik [4]). We show that also the second property fails: adding a zero row/column to a matrix $M \in \cup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ produces a matrix that does not belong to the union $\cup_{r \in \mathbb{N}} \mathcal{K}_{n+1}^{(r)}$ (see Theorem 3).

Motivated by these observations, our focus in this paper is to investigate the following topics: the impact of adding a zero row/column to a matrix in $\cup_{r \in \mathbb{N}} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ (in Section 3), the behavior of the ϑ -rank under some simple graph operations in relation to Conjectures 1 and 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.

1.2. Graphs with Small ϑ -rank Zero or One

In order to investigate the graphs with small $\vartheta\text{-rank}(G) = 0$ or 1, we use the explicit characterizations of the cones $\mathcal{K}_n^{(0)}$ and $\mathcal{K}_n^{(1)}$ provided by Parrilo [25]. 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 $P \geq 0, N \geq 0$ 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 us to show that the bound $\vartheta^{(0)}(G)$ coincides with the bound $\vartheta'(G)$, which is the Lovasz theta number strengthened by adding a nonnegativity constraint (see de Klerk and Pasechnik [4]). Parrilo [25] also shows 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 1); 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, that is, for which M_G belongs to $\mathcal{K}_n^{(0)}$ or $\mathcal{K}_n^{(1)}$. In some cases, it permits us 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 five-cycle has a unique $\mathcal{K}^{(1)}$ -certificate, and this uniqueness property permits us 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 zero as the disjoint unions of cliques, and we reduce the problem of deciding whether a graph has ϑ -rank zero 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 one may produce a graph with ϑ -rank at least two, thus disproving Conjecture 3. We also characterize the maximum number of isolated nodes that can be added to some graphs with ϑ -rank one (such as odd cycles and their complements)

while preserving the ϑ -rank one property (see Section 6). For example, for the graph C_5 , this maximum number of nodes is shown to be equal to eight. Here, too, we exploit uniqueness properties of some of the matrices arising in $\mathcal{K}^{(1)}$ -certificates.

The study of the graphs with ϑ -rank zero 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 recent years. We refer, for example, to Burer and Ye [2], Gökmen and Yildirim [11], and Wang and Kilinç-Karzan [31] (and references therein), which investigate this question for various classes of quadratic problems, such as random instances in Burer and Ye [2] and standard quadratic programs in Gökmen and Yildirim [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 Gvozdenović and Laurent [12, section 6.3]). Hence, also Conjectures 1 and 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 zero comes from its relevance to fundamental questions in complexity theory. Deciding whether a graph G has $\vartheta\text{-rank}(G) = 0$ indeed amounts to deciding whether the polynomial $F_G(x) = (x^{\circ 2})^T M_G x^{\circ 2}$ is a sum of squares, that is, whether an associated semidefinite program is feasible. Equivalently, as mentioned, $\vartheta\text{-rank}(G) = 0$ 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 $P_{ij} \leq -1$ for $\{i, j\} \notin E$, which, thus, again asks about the feasibility of a semidefinite program. Recall that the complexity status of deciding the feasibility of a semidefinite program is still unknown. On the positive side, it is shown in Porkolab and Khachiyan [28] that one can test the 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 is shown in Ramana [29] 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 $\vartheta\text{-rank}(G) = 0$ offers a rich playground to be explored later.

1.3. 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 Parrilo [25], 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 (16) for $\alpha(G)$. In Section 3, we provide explicit constructions showing that adding a zero row/column to a matrix in $\cup_{r \geq 0} \mathcal{K}_n^{(r)} \setminus \mathcal{K}_n^{(0)}$ may produce a matrix in $\text{COP}_{n+1} \setminus \cup_{r \geq 0} \mathcal{K}_{n+1}^{(r)}$, thereby showing strict inclusion $\cup_{r \geq 0} \mathcal{K}_n^{(r)} \subset \text{COP}_n$ 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 Dickinson et al. [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, such as adding an isolated node and deleting an acritical edge, and we investigate their relevance for Conjectures 1 and 2. In Section 5, we discuss the role of critical edges in the study of the graphs with ϑ -rank zero. In particular, we characterize the critical graphs with ϑ -rank zero and give an algorithmic procedure that reduces the problem of deciding whether a graph has ϑ -rank zero 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 one. 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 one property. As a by-product, we show that adding an isolated node can increase the ϑ -rank, thereby refuting Conjecture 3.

1.4. 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, $\chi(G)$ (respectively, $\chi(\overline{G})$) denotes the minimum number of stable sets (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 $M \geq 0$ if it is positive semi-definite (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, that is, 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 1 (Peña et al. [26]). *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*

$$q(x) = \sum_{\substack{I \subseteq [n] \\ |I| \leq d, |I| \equiv d \pmod{2}}} \sigma_I(x) \prod_{i \in I} x_i, \tag{9}$$

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 $P \geq 0$ and scalars $c_{ij} \geq 0$ for $1 \leq i < j \leq n$ such that

$$x^T M x = x^T P x + \sum_{0 \leq i < j \leq n} c_{ij} x_i x_j. \tag{10}$$

This corresponds to the characterization of the cone $\mathcal{K}_n^{(0)}$ given by Parrilo [25], which reads

$$\mathcal{K}_n^{(0)} = \{P + N : P \geq 0, N \geq 0\}. \tag{11}$$

Note that, in (11), 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 $P \geq 0$, $P \leq M$ 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 Equation (10) holds.

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

$$\left(\sum_{i=1}^n x_i \right) x^T M x = \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k. \tag{12}$$

From this, we get the characterization of the cone $\mathcal{K}_n^{(1)}$ from Parrilo [25] (see also de Klerk and Pasechnik [4]).

Lemma 1. *A matrix M belongs to the cone $\mathcal{K}_n^{(1)}$ if and only if there exist matrices $P(i) \geq 0$ for $i \in [n]$ and scalars $c_{ijk} \geq 0$ for $1 \leq i < j < k \leq n$ satisfying Equation (12). Equivalently, there exist matrices $P(i) \in \mathcal{S}^n$ for $i \in [n]$ satisfying the following conditions:*

- i. $P(i) \geq 0$ 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, $M \in \mathcal{K}_n^{(1)}$ if and only if there exist matrices $P(i) \geq 0$ for $i \in [n]$ and scalars $c_{ijk} \geq 0$ satisfying Equation (12). We now obtain conditions (ii)–(iv) by comparing coefficients at both sides of (12). We give the details because they are useful later. First, we start with the left-hand side in (12):

$$\left(\sum_{i=1}^n x_i\right) x^T M x = \sum_{i=1}^n M_{ii} x_i^3 + \sum_{i \neq j \in [n]} x_i^2 x_j (M_{ii} + 2M_{ij}) + \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (M_{ij} + M_{jk} + M_{ik}). \quad (13)$$

Now, we expand the right-hand side in (12):

$$\begin{aligned} \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k &= \sum_{i=1}^n x_i^3 P(i)_{ii} + \sum_{i \neq j \in [n]} x_i^2 x_j (P(i)_{ii} + 2P(i)_{ij}) \\ &+ \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (P(i)_{jk} + P(j)_{ik} + P(k)_{ij} + c_{ijk}). \end{aligned} \quad (14)$$

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

Remark 1. Observe that Lemma 1 remains valid if, in (i), we replace the condition $P(i) \geq 0$ 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 because $\mathcal{S}_+^n \subseteq \mathcal{K}_n^{(0)}$, 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 conditions (i)–(iv) of Lemma 1. 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 Equation (12).

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

Lemma 2. 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 $P \geq 0$ and $N \geq 0$. This implies $Px = 0$ because $P \geq 0$. 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 $M = P + N$. Q.E.D.

Lemma 3. 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 hold:

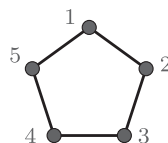
- i. If $x_i > 0$, then $P(i)x = 0$.
- ii. If $x_i, x_j, x_k > 0$, then $M_{ij} + M_{jk} + M_{ik} = P(i)_{ij} + P(j)_{ik} + P(k)_{ij}$.

Proof. By evaluating Equation (12) at x , we get that the left-hand side is zero, whereas 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 $P(i) \geq 0$. On the other hand, if $x_i x_j x_k > 0$, then $c_{ijk} = 0$, which implies the desired identity (see Equations (13) and (14)). Q.E.D.

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

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

Figure 1. Graph C_5 .



The Horn matrix H is known to belong to $\mathcal{K}_n^{(1)}$ (Parrilo [25]). 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:

$$P(1) = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 \end{pmatrix}, \quad P(i) = \begin{pmatrix} \overbrace{1 & 1 & 1}^{i^\pm} & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 \end{pmatrix} \text{ for } i \in [5]. \quad (15)$$

Up to symmetry, it suffices to show that $P(1)$ has this 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 3(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 preceding 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:

$$\frac{1}{\alpha(G)} = \min\{x^T(I + A_G)x : x \in \Delta_n\}. \quad (16)$$

Indeed, we have

$$x^T M_G x = 0 \iff \alpha(G)x^T(A_G + I)x - x^T J x = 0 \iff x^T(A_G + I)x = \frac{1}{\alpha(G)}. \quad (17)$$

The formulation of $\alpha(G)$ in (16) is due to Motzkin and Straus [24] (M-S) and underlies its copositive formulation in (1).

We conclude with recalling the characterization of the minimizers of Problem (16), following Laurent and Vargas [19, corollary 4.4] (see also Gibbons et al. [10]).

Theorem 2. *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 are introduced by Parrilo [25] 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 de Klerk and Pasechnik [4] and Gvozdenović and Laurent [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, whereas $\text{COP}_4 = \mathcal{K}_4^{(0)}$, it is shown in Dickinson et al. [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 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] conjecture 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 $r = 0$

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because $\text{COP}_4 = \mathcal{K}_4^{(0)}$. For $n = 5$ it is shown in Dickinson et al. [7] that the conjecture holds with $r = 1$. Here, we show that this conjecture does not hold for $n \geq 6$. Even more, we give an example of a 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

$$M_1 \oplus M_2 := \left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array} \right), \tag{18}$$

which is clearly copositive. We show as follows 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 4. *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. Q.E.D.

Theorem 3. *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*

$$\left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array} \right) \in \text{COP}_{n+m} \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+m}^{(r)}. \tag{19}$$

Proof. Assume for contradiction $M_1 \oplus M_2 \in \mathcal{K}_n^{(r)}$, that is, 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 4, we obtain that $cp_{M_1}(x)$ is a sum of squares, that is, $M_1 \in \mathcal{K}_n^{(0)}$, yielding a contradiction. Q.E.D.

We now use Theorem 3 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

$$M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)} \Rightarrow \left(\begin{array}{c|c} M & 0 \\ \hline 0 & 0 \end{array} \right) \in \text{COP}_{n+1} \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+1}^{(r)}. \tag{20}$$

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 $n \leq 4$ (Diananda [5]). The situation for the case of 5×5 matrices remains open.

Question 1. Does equality $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ hold?

Dickinson et al. [7] prove that any 5×5 copositive matrix with 0,1-valued diagonal entries belongs to $\mathcal{K}_5^{(1)}$. They conjecture 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 Dickinson et al. [7, conjecture 1]). Using Theorem 3, we can disprove this conjecture.

Example 2. Let $M_1 := M_{C_5} = H$ be the Horn matrix, known to be copositive with $H \notin \mathcal{K}_n^{(0)}$. 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, we obtain

$$\left(\begin{array}{c|c} H & 0 \\ \hline 0 & 0 \end{array} \right) \in \text{COP}_6 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_6^{(r)}, \quad \left(\begin{array}{c|cc} H & & 0 \\ \hline & 1 & -1 \\ 0 & -1 & 1 \end{array} \right) \in \text{COP}_7 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_7^{(r)}. \tag{21}$$

The leftmost matrix in (21) 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 $n \geq 6$.

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The rightmost matrix in (21) is copositive, has all its diagonal entries equal to one, 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 one for any size $n \geq 7$. In contrast, as mentioned, Dickinson et al. [7] prove 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 2. 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 Laurent and Vargas [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. 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, we have

$$M := \left(\begin{array}{c|cc} M_1 & & 0 \\ \hline & 1 & -1 \\ 0 & -1 & 1 \end{array} \right) \in \text{COP}_{n+2} \setminus \bigcup_{r \geq 0} \mathcal{K}_{n+2}^{(r)}. \quad (22)$$

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 $x^T M x$ 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, 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 $\mathcal{K}_5^{(1)}$ (Dickinson et al. [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. 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 is observed in Example 1.

Theorem 4. 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:

$$d_{i-1}d_i + d_i d_{i+1} \geq d_{i-1}d_{i+1} \text{ for } i \in [5] \text{ (indices taken modulo 5)}. \quad (23)$$

Proof. Set $M := DHD$. First, we show the “if” part. Assume d_1, \dots, d_5 satisfy Conditions (23); 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 (15); we show that the matrices $Q(i)$ form a $\mathcal{K}^{(1)}$ -certificate for M , that is, satisfy the conditions (i)–(iv) from Lemma 1. Clearly, $Q(i) \geq 0$ and $Q(i)_{ii} = d_i^2$ for all $i \in [5]$, so (i) and (ii) hold. Also, $2Q(i)_{ij} + Q(j)_{ii} = 2d_i d_j P(i)_{ij} + d_i^2 P(j)_{ii} = 2M_{ij} + M_{ii}$ because $P(i)_{ij} = H_{ij}$ and $P(j)_{ii} = H_{ii}$, so (iii) holds. We now check (iv), that is, $Q(i)_{jk} + Q(j)_{ik} + Q(k)_{ij} \leq M_{ij} + M_{jk} + M_{ik}$ 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

$$\begin{aligned} M_{12} + M_{25} + M_{15} - (Q(5)_{12} + Q(1)_{25} + Q(2)_{15}) \\ &= d_1d_2 - d_2d_5 + d_1d_5 - (d_1d_2P(5)_{12} + d_2d_5P(1)_{25} + d_1d_5P(2)_{15}) \\ &= d_1d_2 - d_2d_5 + d_1d_5 - (-d_1d_2 + d_2d_5 - d_1d_5) \\ &= 2(d_1d_2 - d_2d_5 + d_1d_5), \end{aligned}$$

which is nonnegative if and only if (23) holds. Hence, Conditions (23) indeed imply that condition (iii) of Lemma 1 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 (15). In view of the preceding, this implies that the d_i 's satisfy Conditions (23) as desired. Up to symmetry, it suffices to show $Q(1) = DP(1)D$. For this, note that, if $z^T Hz = 0$ for $z \in \mathbb{R}_+^n$, then $y^T My = 0$ for $y := D^{-1}z \in \mathbb{R}_+^n$ and, thus, by Lemma 3, $Q(i)y = 0$ 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 $x^T Hx$, and the corresponding vectors $y_i = D^{-1}z_i$ for $i = 1, 2, 3, 4$, which are zeros of $x^T Mx$. Let C_1, \dots, C_5 denote the columns of $Q(1)$. Then, using the zeros y_1, \dots, y_5 of $x^T Mx$, 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 $\frac{C_1}{d_1} = \frac{C_2}{d_2} = \frac{C_3}{d_3} = -\frac{C_4}{d_4}$. As $Q(1)_{11} = d_1^2$ one easily deduces $Q(1) = DP(1)D$ as desired. Q.E.D.

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 critical edges and their impact on Conjectures 1 and 2. In particular, we show that it suffices to show Conjectures 1 and 2 for the class of critical graphs and that Conjecture 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 use later on.

Lemma 5. *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, $M_G \in \mathcal{K}^{(\alpha)}$ implies $M_H \in \mathcal{K}^{(\alpha)}$. \square

Remark 2. Let G be the graph obtained by adding a pendant edge to C_5 (see the leftmost graph in Figure 3) so that $\alpha(G) = 3 = \alpha(C_5) + 1$. Then, G has ϑ -rank zero as it can be covered by $\alpha(G) = 3$ cliques. However, C_5 is an induced subgraph of G and has ϑ -rank one (see Example 1). This shows that the condition of having the same stability number in Lemma 5 cannot be dropped.

4.1. Role of Isolated Nodes

We recall a result from Gvozdenović and Laurent [12] that 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 1 (Gvozdenović and Laurent [12]). *For any graph $G = (V, E)$, we have*

$$\vartheta\text{-rank}(G) \leq 1 + \max_{i \in V} \vartheta\text{-rank}((G \setminus i^\perp) \oplus i). \tag{24}$$

In view of Proposition 1, understanding how adding isolated nodes changes the ϑ -rank is crucial for Conjectures 1 and 2. On the one hand, it is shown in Gvozdenović and Laurent [12] that, if adding an isolated node does not increase the ϑ -rank, then Conjecture 1 holds.

Proposition 2 (Gvozdenović and Laurent [12]). *Assume $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G)$ for any graph G . Then, Conjecture 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 2.

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Proposition 3. Let $a \in \mathbb{N}$. 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 1 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 $\vartheta\text{-rank}(G) \leq a + 1 + (a + 1)(\alpha(G) - 1) - 1 = (a + 1)\alpha(G) - 1$. Q.E.D.

On the other hand, as we now show, Conjecture 2 holds if and only if the ϑ -rank remains finite after adding isolated nodes to finite ϑ -rank graphs.

Proposition 4. Conjecture 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. Assume that $\vartheta\text{-rank}(G) < \infty$ implies $\vartheta\text{-rank}(G \oplus i_0) < \infty$. Assume also that Conjecture 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 1, 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 $G \setminus i^\perp \oplus i$ is a counterexample with fewer 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. Q.E.D.

Clearly, if G has an isolated node i_0 , then $G \setminus i_0 \oplus i_0 = G$, and thus, the result in Proposition 1 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 Gvozdenović and Laurent [12]) points out the difficulty of analyzing the ϑ -rank of graphs with isolated nodes. We investigate this question in Section 6.2.

On the other hand, adding an isolated node to a graph with $\vartheta\text{-rank} = 0$ preserves the property of having $\vartheta\text{-rank} = 0$. 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 (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 (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 zero property, the next result follows as a direct application of Proposition 1.

Lemma 6 (de Klerk and Pasechnik [4]). If $\vartheta\text{-rank}(G \setminus i^\perp) = 0$ for all $i \in V$, then $\vartheta\text{-rank}(G) \leq 1$.

Example 4. As an application of Lemma 6, we obtain that $\vartheta\text{-rank}(C_{2n+1}) \leq 1$ and $\vartheta\text{-rank}(\overline{C_{2n+1}}) \leq 1$. 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 zero. Hence, by Lemma 6, $\vartheta\text{-rank}(G) \leq 1$, and thus, Conjecture 1 holds for graphs with $\alpha(G) = 2$ (as shown in de Klerk and Pasechnik [4]).

Let $G = C_5 \oplus i_0$ be the graph obtained by adding one isolated node to the five-cycle. As shown in de Klerk and Pasechnik [4], G has ϑ -rank one, and the graph $G \setminus i_0^\perp$ is the five-cycle that also has ϑ -rank one. This shows that Lemma 6 does not permit us to characterize, in general, graphs with ϑ -rank one. For details on the impact of adding isolated nodes to C_5 , see Corollary 2.

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 noncritical edges can only increase the ϑ -rank. On the other hand, we can strengthen a result from Gvozdenović and Laurent [12] for the class of acritical graphs.

Lemma 7 (Laurent and Vargas [19]). Let $G = (V, E)$ be a graph and let $e \in E$. If e is not a critical edge, that is, $\alpha(G) = \alpha(G \setminus e)$, then $\vartheta\text{-rank}(G) \leq \vartheta\text{-rank}(G \setminus e)$. Hence, it suffices to show Conjectures 1 and 2 for the class of critical graphs.

Remark 3. Let $G = (V, E)$ be a graph. Then, one can find a subgraph $H = (V, F)$ of G (with $F \subseteq E$) that 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 noncritical edge until getting a subgraph in which all edges are critical. Then, by Lemma 7, for any such H , we have

$$\vartheta\text{-rank}(G) \leq \vartheta\text{-rank}(H). \tag{25}$$

In this lemma, it is observed that critical edges play a role in the study of the ϑ -rank, namely, it suffices to bound the ϑ -rank of critical graphs. On the other hand, we now prove a stronger version of Conjecture 1 for acritical

graphs with $\alpha(G) \leq 8$. In Gvozdenović and Laurent [12], the authors propose the following conjecture and proved that it implies Conjecture 1.

Conjecture 5 (Gvozdenović and Laurent [12]). *For any $r \geq 1$, we have*

$$\vartheta^{(r)}(G) \leq r + \max_{S \subseteq V, S \text{ stable}, |S|=r} \vartheta^{(0)}(G \setminus S^\perp). \tag{26}$$

Theorem 5 (Gvozdenović and Laurent [12]). *Conjecture 5 holds for $r \leq \min(6, \alpha(G) - 1)$ and for $r = 7 = \alpha(G) - 1$. In particular, Conjecture 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 5. *Let G be an acritical graph with $\alpha(G) \leq 8$. Then, $\vartheta\text{-rank}(G) \leq \alpha(G) - 2$.*

Proof. It suffices to show that $\vartheta^{(0)}(G \setminus S^\perp) \leq 2$ if S is stable of size $\alpha(G) - 2$ because then the result follows from Equation (26). 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 (Chudnovsky et al. [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 preceding argument. Thus, we reach a contradiction because 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. Toward Characterizing Graphs with ϑ -rank Zero

In this section, we investigate the graphs G with ϑ -rank zero, that is, such that $\vartheta^{(0)}(G) = \alpha(G)$ or, equivalently, $M_G \in \mathcal{K}_n^{(0)}$. Recall the well-known “sandwich inequality” from Lovász [22]:

$$\alpha(G) \leq \vartheta'(G) = \vartheta^{(0)}(G) \leq \vartheta(G) \leq \overline{\chi}(G). \tag{27}$$

In view of (27), if G can be covered by $\alpha(G)$ cliques, then G has ϑ -rank zero. In addition, if $\alpha(G) = \alpha$ and $V_1, V_2, \dots, V_\alpha$ are cliques partitioning V , then the matrix

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

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 graphs with $\alpha(G) \leq 2$. We also provide an algorithmic method that permits us to reduce the characterization of ϑ -rank zero 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 Zero

The next result is repeatedly used.

Lemma 8. *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. The proof follows directly from Lemma 2 because $(\chi^S)^T M_G \chi^S = 0$ as $\chi^S / |S|$ is a global minimizer of (16) (recall (17)). Q.E.D.

Proposition 6. *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 $\vartheta\text{-rank}(G) = 0$, then each connected component of the graph G_c is a clique of G .*

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Proof. By assumption, $\vartheta\text{-rank}(G) = 0$. 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 8, 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:

$$P = \begin{pmatrix} (\alpha - 1)J_{|V_1|} & a_{12}J_{|V_1| \times |V_2|} & \cdots & a_{1p}J_{|V_1| \times |V_p|} \\ a_{21}J_{|V_2| \times |V_1|} & (\alpha - 1)J_{|V_2|} & \cdots & a_{2p}J_{|V_2| \times |V_p|} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1}J_{|V_p| \times |V_1|} & a_{p2}J_{|V_p| \times |V_2|} & \cdots & (\alpha - 1)J_{|V_p|} \end{pmatrix} \quad (28)$$

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 nonedges. Hence, we show that each component V_i is a clique of G , which concludes the proof. \square

Corollary 1. Assume $G = (V, E)$ is a critical graph, that is, all its edges are critical. Then, we have $\vartheta\text{-rank}(G) = 0$ if and only if G is the disjoint union of $\alpha(G)$ cliques. In particular, we have $\vartheta\text{-rank}(G) = 0$ if and only if $\bar{\chi}(G) = \alpha(G)$.

Proof. The “only if” part follows from Proposition 6, and the “if” part follows from Equation (27). The last claim follows directly. \square

Example 5. Let $n \geq 2$. We see in Remark 3 that $\vartheta\text{-rank}(C_{2n+1}) \leq 1$ and $\vartheta\text{-rank}(\overline{C_{2n+1}}) \leq 1$. Here, we can show, as an application of Corollary 1, that their $\vartheta\text{-rank}$ is equal to one.

- C_{2n+1} is critical and connected (and not a clique), and thus, by Corollary 1, $\vartheta\text{-rank}(C_{2n+1}) \geq 1$.
- 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, $\vartheta\text{-rank}(\overline{C_{2n+1}}) \geq 1$.

Next, we give an example of an acritical graph with $\vartheta\text{-rank}$ one.

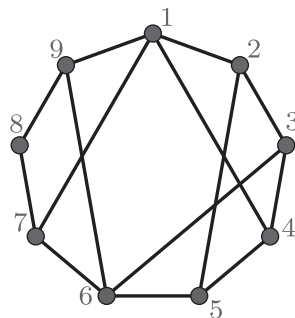
Example 6. Consider the graph H_9 from Figure 2. Note that $\alpha(H_9) = 4$ and that C_9 is a critical subgraph of H_9 with the same stability number. Hence, by Remark 3, $\vartheta\text{-rank}(H_9) \leq \vartheta\text{-rank}(C_9) = 1$.

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 four in H_9 , by applying Lemma 8, 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 because $P_{16} \leq -1$ as $\{1, 6\}$ is a nonedge.

Figure 2. Graph H_9 , acritical.



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

Here, we observe that the result of Corollary 1 holds for all (not necessarily critical) graphs with $\alpha(G) \leq 2$. In Section 5.4, we show that this also holds for acritical graphs with $\alpha(G) \geq |V| - 4$ (see Proposition 7).

Lemma 9. *Let G be a graph with $\alpha(G) \leq 2$. Then, $\vartheta\text{-rank}(G) = 0$ if and only if $\bar{\chi}(G) = \alpha(G)$.*

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 $\vartheta\text{-rank}$ one (see Example 5). This contradicts Lemma 5, which claims that, for every induced subgraph H with $\alpha(H) = \alpha(G)$, we must have $\vartheta\text{-rank}(H) \leq \vartheta\text{-rank}(G)$. Q.E.D.

Example 7. We give some examples showing that the characterization in Corollary 1 and Lemma 9 of rank zero graphs as those with $\bar{\chi}(G) = \alpha(G)$ does not hold if $\alpha(G) \geq 3$ and G has some noncritical edges.

Let G be the Petersen graph. Then, G has rank zero because $\vartheta(G) = \vartheta^{(0)}(G) = \alpha(G) (= 4)$, but $\bar{\chi}(G) = 5 > \alpha(G) = 4$ (see Lovász [22]). Note that the Petersen graph is, in fact, acritical. The graph $G = \overline{G_{13}}$ considered in Mancinska and Roberson [23] provides another example with $3 = \alpha(G) = \vartheta(G) < \bar{\chi}(G) = 4$ 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 that $G_{n,k}$ has as a vertex set the collection of all k -subsets of $[n]$, in which two vertices are adjacent if the corresponding subsets are disjoint. Note that $G_{5,2}$ is the Petersen graph. It is shown by Lovász [21, 22] that

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

Therefore, $\vartheta\text{-rank}(G_{n,k}) = 0$. However, $\bar{\chi}(G_{n,k}) \geq \binom{n}{k} / \lfloor n/k \rfloor > \binom{n-1}{k-1} = \alpha(G_{n,k})$ 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 prove 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 $\vartheta\text{-rank}$ Zero Graphs to the Class of Acritical Graphs

Here, we further investigate the structure of graphs with $\vartheta\text{-rank}$ zero. We introduce a reduction procedure, which we use to reduce the task of checking the $\vartheta\text{-rank}$ zero property to the same property for the class of acritical graphs. This procedure relies on the following graph construction, which is motivated by Lemma 6.

Definition 1. 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 $\vartheta\text{-rank}$ zero property and the stability number.

Lemma 10. *Assume G is a graph with $\vartheta\text{-rank}(G) = 0$ and let $\Gamma(G)$ be the graph as in Definition 1. 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 6), 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 $P \geq 0, N \geq 0$ and $P_{ii} = \alpha - 1$ for all $i \in V$. As shown in the proof of Lemma 6, the matrix P has the block form (28) with respect to the partition $V = V_1 \cup \dots \cup V_p$. Then, the following $p \times p$ matrix

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

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is positive semidefinite. We show that $P' \leq M_{\Gamma(G)}$, thus proving that $\Gamma(G)$ has ϑ -rank zero. As $P' \geq 0$, 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). 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. Q.E.D.

Lemma 11. Assume ϑ -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 $\cup_{i \in C} C_i$ 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 10). □

Now, we provide a partial converse to the result of Lemma 10.

Lemma 12. 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 1. If ϑ -rank($\Gamma(G)$) = 0 and $\alpha(\Gamma(G)) \leq \alpha(G)$, then we have ϑ -rank(G) = 0.

Proof. By assumption, ϑ -rank($\Gamma(G)$) = 0. Hence, there exists a matrix $P \geq 0$ 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, $P' \geq 0$. We claim that $P' \leq M_G$ holds. This is true for the diagonal entries and for the positions corresponding to edges of G (because 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, $a_{ij} \leq -1$ because $P \leq M_{\Gamma(G)}$. □

So we show that, if we apply the Γ -operator to a graph G with ϑ -rank zero, then we obtain a new graph $\Gamma(G)$ with ϑ -rank zero 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 2. 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 10 and 11, we obtain the following result.

Lemma 13. Let G be a graph with ϑ -rank(G) = 0 and let $R(G)$ be its residual graph as defined in Definition 2. 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 these results, we now present an algorithmic procedure that permits us to reduce the task of checking whether a graph has ϑ -rank zero to the same task restricted to the class of graphs with no critical edges.

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Algorithm 1 (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 \Leftrightarrow 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 this algorithm. For this, let us assume the algorithm does not output ϑ -rank(G) ≥ 1 . In view of Definition 2, 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 $\alpha(R(G)) = \alpha(G)$. It 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 10, and the “if” part follows using Lemma 12.

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

Theorem 6. For any fixed integer α , the problem of deciding whether a graph with stability number α has ϑ -rank zero is reducible in polynomial time to the problem of deciding whether a graph with no critical edges and stability number α has ϑ -rank zero.

Example 8. 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.

Remark 4. The results from this section can be adapted to the Lovász parameter $\vartheta(G)$ instead of $\vartheta^{(0)}(G)$. Recall from Lovász [22] 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 Zero

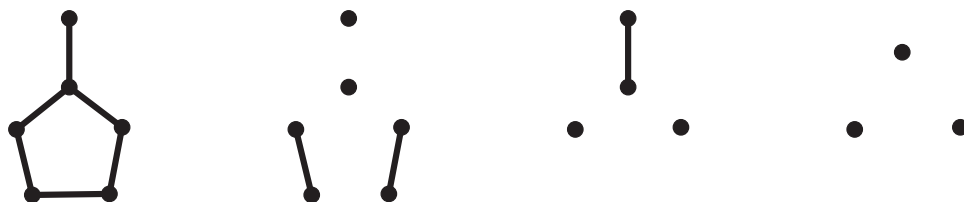
Motivated by the reduction to acritical graphs from the previous section, we now consider acritical graphs with a large stability number. We show that, if $G = (V, E)$ is acritical with $\alpha(G) \geq |V| - 4$, then V can be covered by $\alpha(G)$ cliques, and thus, G has ϑ -rank zero.

Proposition 7. Let $G = (V, E)$ be a graph and assume $\alpha(G) \geq |V| - 4$.

- i. If $\alpha(G) \geq |V| - 2$, then $\overline{\chi}(G) = \alpha(G)$, and thus, ϑ -rank(G) = 0.
- ii. If $\alpha(G) = |V| - 3$, then $\overline{\chi}(G) = \alpha(G)$, 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 $\overline{\chi}(G) = \alpha(G)$, and thus, ϑ -rank(G) = 0.

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

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



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

We claim that G is perfect. 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 three vertices of H , this implies $\alpha(G) \leq |V| - 3$, yielding a contradiction.

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

Let S be an α -stable set and set $V \setminus S = \{x, y, z\}$. Assume G is not covered by α cliques, and we show that G is the disjoint union of C_5 and $n - 5$ isolated vertices. As $\overline{\chi}(G) \neq \alpha(G)$, 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. Assume $\alpha(G) = |V| - 4$ 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 is 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 [13] theorem, there exists $W \subseteq T$ such that $|N_S(W)| \leq |W| - 1$. Then, $|W| \geq 3$ because $|N_S(W)| \geq 2$. 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 $\overline{\chi}(G) = \alpha(G)$. So we now assume that $N_S(w) = \{u, v\}$. Note that $\overline{\chi}(G) = \alpha(G)$ holds in each of the following two cases: (i) when T contains a clique of size three (say, $\{x, y, z\}$) and (ii) when T contains two disjoint edges (say, $\{x, y\}, \{z, w\} \in E$) because, then, G is covered by the cliques $\{x, y, z, u\}$, $\{v, w\}$ in case (i) or by the cliques $\{x, y, u\}$, $\{z, w, v\}$ 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 or 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 that is C_{2k+1} or $\overline{C_{2k+1}}$ 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 that H cannot be $\overline{C_7}$ because $\alpha(\overline{C_7}) = 2$, whereas 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 five-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 (to t), then G is covered by the cliques $\{x, u\}$, $\{y, z, t\}$, $\{w, v\}$ ($\{y, z, v\}$, $\{w, t\}$) 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 five-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 $S \setminus \{u, v, t\}$.

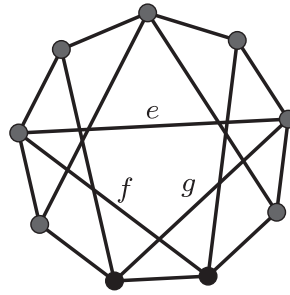
This concludes the proof. Q.E.D.

Remark 5.

(i) As we just see in Proposition 7(ii), the only graphs G with $\alpha(G) = |V| - 3$ that do not have ϑ -rank zero 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 show that $\vartheta\text{-rank}(C_5 \oplus \overline{K_{n-5}}) = 1$ if and only if $n \leq 13$ (see Corollary 2 in Section 6.2).

(ii) Proposition 7 shows that any acritical graph with $\alpha(G) \geq |V| - 4$ satisfies $\overline{\chi}(G) = \alpha(G)$ and, thus, has ϑ -rank zero. The same holds for graphs with $\alpha(G) = 2$ (Lemma 9). The next natural case to consider are graphs with $\alpha(G) = 3$ and $n \geq 8$ nodes. Polak [27] verifies (using a computer) that, if G is an acritical graph on eight nodes with

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



$\alpha(G) = 3$, then $\bar{\chi}(G) = \alpha(G)$ holds (and, thus, $\vartheta\text{-rank}(G) = 0$). In addition, if G is acritical on nine 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 $\vartheta\text{-rank}$ zero.

(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 nonisomorphic acritical graphs on nine vertices that have $\vartheta\text{-rank}$ at least one (and, thus, cannot be covered by $\alpha(G)$ cliques). Polak [27] verifies (using a computer) that these are the only nonisomorphic acritical graphs on nine vertices that do not have $\vartheta\text{-rank}$ zero.

(iv) Finally, we use the graph H_9 from Example 6 to construct a class of acritical graphs with $\bar{\chi}(\bar{G}) > \alpha(G)$ 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 $\vartheta\text{-rank}(G) = \vartheta\text{-rank}(H_9 \oplus \bar{K}_{\alpha-4})$. 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 $\vartheta\text{-rank}$

As mentioned in Proposition 2, if the $\vartheta\text{-rank}$ does not increase under the simple graph operation of adding an isolated node, then Conjecture 1 holds. In Gvozdenović and Lauren [12], it is conjectured that adding isolated nodes indeed does not increase the $\vartheta\text{-rank}$. In this section, we investigate this question and, in fact, disprove the latter conjecture already for graphs with $\vartheta\text{-rank}$ one. 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 $\vartheta\text{-rank}$ one. Then, we investigate the impact of adding isolated nodes to certain classes of graphs H with $\vartheta\text{-rank}$ one. 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 although preserving the $\vartheta\text{-rank}$ one property (Theorem 7). Second, we show that adding this number of isolated nodes indeed produces a graph with $\vartheta\text{-rank}$ one when H satisfies the property $\vartheta\text{-rank}(H \setminus i^\perp) = 0$ for all its nodes (Theorem 8). 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 although preserving the $\vartheta\text{-rank}$ one property (see Corollary 2). As a by-product, we obtain that adding an isolated node to a graph with $\vartheta\text{-rank}$ one can produce a graph with $\vartheta\text{-rank} \geq$ two. For instance, $C_5 \oplus \bar{K}_8$ has $\vartheta\text{-rank} 1$, but $C_5 \oplus \bar{K}_9$ has $\vartheta\text{-rank}$ two.

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

The following results are based on the kernel property observed in Lemma 3, which applies to the matrices M_G and permits us to exploit the structure of the graph G .

Lemma 14. 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 hold:

- i. If S is a stable set of size $\alpha(G)$ and $i \in S$, then we have $\sum_{j \in S} C_j = 0$.

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- 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

$$P(i) = \left(\begin{array}{c|c} (\alpha - 1)J_{|i^\perp|} & -1 \\ \hline -1 & \frac{1}{\alpha - 1}J_{|V \setminus i^\perp|} \end{array} \right), \tag{29}$$

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 3(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 Equation (17) and Theorem 2). Using Lemma 3(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 $P(i)$. Q.E.D.

Using Lemma 14, we can show that, for some \mathcal{D} -rank one graphs, the construction of the matrices $P(i)$ in a $\mathcal{K}^{(1)}$ -certificate is in fact unique. We already see that this is the case for the five-cycle in Example 1, and 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.

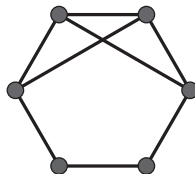
Example 9. Let $G = (V, E)$ be a critical graph with $\alpha(G) = 2$. Then, $M_G \in \mathcal{K}^{(1)}$ (recall Theorem 5). Let $\{P(i) : i \in V\}$ be a $\mathcal{K}^{(1)}$ -certificate for M_G . We show that the matrices $P(i)$ are uniquely determined using Equation (29). Indeed, as $\alpha(G) = 2$, 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 14 can be applied, and we obtain that, for every $i \in V$, the matrix $P(i)$ takes the form (29).

Example 10. 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 14, we conclude that the matrix $P(i_0)$ takes the form (29) (also displayed as follows). In particular, we have $P(i_0)_{ij} = 1/2$ and $P(i_0)_{i_0 i} = -1$ 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 14(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 14(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 1, 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 14(i), we obtain that the columns indexed by 1, 3, and i_0 sum up to zero, which enables to complete the rest of the matrix $P(1)$, whose shape is shown as follows.

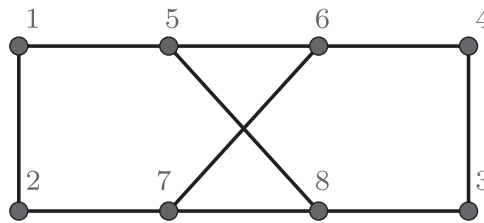
$$P(i_0) = \begin{array}{c} i_0 \quad [5] \\ \begin{pmatrix} 2 & -1 \\ -1 & 1/2 \end{pmatrix} \end{array}, \quad P(1) = \begin{array}{c} i_0 \quad \{3, 4\} \quad \{1, 2, 5\} \\ \begin{pmatrix} 2 & -7/4 & -1/4 \\ -7/4 & 7/2 & -7/4 \\ -1/4 & -7/4 & 2 \end{pmatrix} \end{array}.$$

Figure 5. A critical graph with stability number two.



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



Lemma 15. 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, there exists $x \in \Delta_n$ such that $x^T M_G x = 0$ and $\text{Supp}(x) = S$. Then, Lemma 3(ii) gives the desired result. Q.E.D.

Example 11. 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 is verified numerically in Peña et al. [26]). 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 14, the matrices $P(1), P(2), P(3)$, and $P(4)$ take the form (29), 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 15, one should have $P(1)_{23} + P(2)_{13} + P(3)_{12} = 3 \times 1 - 3 = 0$, so we reach a contradiction.

Consider the graph H_8 , shown in Figure 7. 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 eight nodes with $\vartheta\text{-rank} = 2$. To see this, one can use the list of critical graphs on eight nodes from Small [30] and verify that all of them have $\vartheta\text{-rank}$ at most one except G_8 and H_8 . Note also that, as observed in Peña et al. [26], any graph with at most seven nodes has $\vartheta\text{-rank}$ at most one.

6.2. Adding Isolated Nodes to Graphs with $\vartheta\text{-rank}$ One

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

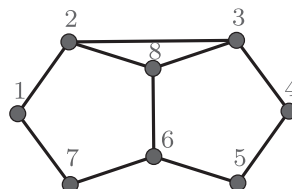
Throughout this section, we consider a graph of the form $G = H \oplus \overline{K_{\alpha-k}}$, where $H = (V, E)$ has $\alpha(H) =: k$ so that $\alpha(G) = \alpha$. Here, α and k are integers such that $\alpha \geq k \geq 2$. Note that, if $k = 1$, then H is a clique, and thus, G has $\vartheta\text{-rank}$ 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 7. 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

$$\alpha \leq \frac{k(k+3)}{k-1} = k + 4 + \frac{4}{k-1}. \tag{30}$$

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



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The rest of the section is devoted to the proof of Theorem 7. Throughout, we assume that G and H are as defined in Theorem 7, so $M_G = \alpha(A_G + I) - J \in \mathcal{K}_n^{(1)}$. We 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 8 (Dobre and Vera [8]). *Assume $M \in \mathcal{K}_n^{(1)}$. 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 8. In particular, since any permutation $\sigma \in \text{Sym}(W)$ of the isolated nodes leaves the graph G invariant, it follows that

$$\sigma(P(i)) = P(\sigma(i)), \text{ i.e., } P(i)_{\sigma(j)\sigma(k)} = P(\sigma(i))_{jk} \text{ for all } \sigma \in \text{Sym}(W) \text{ and } j, k \in V \cup W. \quad (31)$$

We use this symmetry property repeatedly in the proof. We mention a simple identity that follows as a direct application of Lemma 15, which we also repeatedly use in the rest of the section:

$$P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = -3 \text{ if } \{i, j, k\} \text{ is contained in a stable set of } G \text{ with size } \alpha(G). \quad (32)$$

Now, we prove some preliminary lemmas, and we end with Lemma 19, which directly implies Theorem 7. We start with a general property about the structure of the submatrices $P(i)[W]$ when $i \in W$ is an isolated node.

Lemma 16. *There exists a scalar $b \in \mathbb{R}$ such that the following hold:*

- 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 (31), 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 1, we have $P(i)_{jj} + 2P(j)_{ij} = \alpha - 3$, which implies $P(i)_{jj} = \alpha - 2b - 3$, and thus, (ii) holds. Using again (31) with $\sigma = (i, k)$, we obtain $P(i)_{\sigma(i)\sigma(j)} = P(\sigma(i))_{ij}$, 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 Equation (32) for the nodes i, j, k , we obtain $P(i)_{jk} = P(j)_{ik} = P(k)_{ij} = -1$, thus showing (iii). Q.E.D.

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

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

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 14(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 Equation (31) 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.

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For this, consider an α -stable set S of G . Then, $i \in S$, and thus, by Lemma 14(i), the columns of $P(i)$ indexed by S sum up to zero. Using the identities of Lemma 16 combined with the preceding facts on the remaining entries of $P(i)$, we obtain

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

This concludes the proof. Q.E.D.

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

Lemma 18. Assume H_c is connected. For any $v \in V$, the submatrix $P(v)[W \cup \{v\}]$ takes the form

$$P(v)[W \cup \{v\}] = \left(\begin{array}{c|c} M_b & \begin{matrix} \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \\ \alpha - 1 \end{matrix} \\ \hline \begin{matrix} \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \\ \alpha - 1 \end{matrix} & \alpha - 1 \end{array} \right), \tag{33}$$

where the blocks are indexed by W and $\{v\}$, respectively. Here, $b \in \mathbb{R}$ is the constant from Lemma 16, and the matrix M_b is indexed by V and takes the form

$$M_b = \begin{pmatrix} a & c & \cdots & c \\ c & a & \cdots & c \\ \vdots & \vdots & \ddots & \vdots \\ c & c & \cdots & a \end{pmatrix}, \quad \text{with } a = \alpha - 3 - \frac{2}{k}(b(k + 1) + 1 - \alpha - b\alpha), \quad c = -1 - \frac{2}{k}(b + 1). \tag{34}$$

Proof. Consider an isolated node $i \in W$. By Lemma 1, 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 (32), 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 1, 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. Q.E.D.

The following lemma gives necessary and sufficient conditions for the matrix in Equation (33) to be positive semidefinite. In particular, part (ii) of the lemma shows Theorem 7.

Lemma 19. The matrix in Equation (33) 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 (33) with respect to its (v, v) -entry, we obtain that $P(v)[W \cup \{v\}] \geq 0$ if and only if

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

This happens if and only if $a \geq c$ 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

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

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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

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

after canceling terms in the right-hand side. Canceling 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 7, we see 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 one, then the parameters α and k must satisfy Inequality (30). 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 one 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 one property. Hence, for these graphs, we characterize the exact number of isolated nodes that can be added while preserving the ϑ -rank one property.

We begin with a preliminary lemma that we use for our main result.

Lemma 20. Assume $\alpha \geq k \geq 2$ satisfy Inequality (30), and let $M := \alpha I_{\alpha - k} - J_{\alpha - k}$. Then,

$$\left(\begin{array}{c|c} M & \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \\ \hline \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & \alpha - 1 \end{array} \right) \geq 0.$$

Proof. The matrix corresponds to the matrix in Equation (33) with $b = -1$, which gives $a = \alpha - 1$ and $c = -1$ so that $M = M_b = M_{-1}$. As $a \geq c$, using Lemma 19, we get the desired result. \square

Theorem 8. 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 Inequality (30). 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 1. Recall Remark 1 in which we observe that it suffices to show that the matrices $P(i)$ belong to the cone $\mathcal{K}^{(0)}$. For this, consider the following construction (inspired from Gvozdenović and Laurent [12]), in which 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 $P(i) \geq 0$ 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 $Q(i) \geq 0$ and $R(i) \in \mathcal{K}^{(0)}$.

First, we show that $Q(i)$ is positive semidefinite. By Lemma 20, we know that the submatrix $Q(i)[W \cup i^\perp]$ is positive semidefinite. We 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 $Q(i) \geq 0$. Namely, one can show $C_v = \frac{1}{1-k} (\sum_{j \in W} C_j + C_i) =: C$ by direct inspection of the following entries:

- For the entries indexed by $u \in I$, we have

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

- For the entries indexed by $u \in i^\perp$, we have

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

- And 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 conjecture, $M_{H \setminus i^\perp} \in \mathcal{K}^{(0)}$. Since adding zero row/columns preserves 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 1 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 $P(u)_{vv} + 2P(v)_{uv} = \frac{\alpha^2}{k} - 1 + 2 \left(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k} \right) = \alpha - 3$.

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 $P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = -3$,

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- 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. Q.E.D.

We now give some examples of graphs for which the conditions of Theorem 7 and 8 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 one.

Corollary 2. For any integer $n \geq 2$, the following hold:

- i. ϑ -rank($\overline{C_{2n+1}} \oplus \overline{K_m}$) = 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, H satisfies the property ϑ -rank($H \setminus i^\perp$) = 0 for all $i \in V$, and thus, the assumption of Theorem 8 holds. For $H = C_{2n+1}$, Inequality (30) 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) and (ii) follows as a direct application of Theorem 8.

The “only if” part in both (i) and (ii) follows as a direct application of Theorem 7 because the graph C_{2n+1} is critical, whereas the subgraph of critical edges of $\overline{C_{2n+1}}$ is a connected graph. □

Corollary 3. 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 8. 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 $H_0 = C_{2n+1}$ ($n \geq 2$) 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 5, ϑ -rank($H \oplus \overline{K_m}$) $\geq \vartheta$ -rank($H_0 \oplus \overline{K_m}$) ≥ 2 , where the last inequality follows from Corollary 2. Q.E.D.

Corollary 4. 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 hold:

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

Proof. By Corollary 1, we know ϑ -rank(H_0) ≥ 1 . Pick a stable set $W \subseteq V(H \setminus H_0)$ such that $\alpha(H_0 \oplus W) = \alpha(H)$, that is, $|W| = \alpha(H) - \alpha(H_0)$. Then, $H_0 \oplus W$ is an induced subgraph of H with the same stability number as H . Then, by Lemma 5, ϑ -rank($H_0 \oplus W \oplus \overline{K_s}$) $\leq \vartheta$ -rank($H \oplus \overline{K_s}$) for any $s \geq 0$. By applying Corollary 3 to the graph H_0 , we obtain that ϑ -rank($H_0 \oplus W \oplus \overline{K_s}$) ≥ 2 if $s + |W| \geq 9$. From these facts, (i) and (ii) now follow easily. Q.E.D.

7. Concluding Remarks

In this paper, we make some new contributions about the hierarchy of semidefinite relaxations of the copositive cone COP_n provided by Parrilo’s cones $\mathcal{K}_n^{(r)}$. In particular, we give a construction for matrices in COP_6 that do not belong to any cone $\mathcal{K}_6^{(r)}$; this shows that the union of the cones $\mathcal{K}_n^{(r)}$ does not cover the full copositive cone COP_n for $n \geq 6$. The question of whether this result extends to the case $n = 5$ remains open. We investigate this question in (Laurent and Vargas [20]), in which we show that the question of deciding whether $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ reduces to deciding whether any positive diagonal scaling of the Horn matrix lies in some cone $\mathcal{K}_5^{(r)}$.

Whereas it is shown in Dickinson et al. [7] that any 5×5 copositive matrix with an all-ones diagonal belongs to $\mathcal{K}_5^{(1)}$, we show that there exist matrices in COP_7 with an all-ones diagonal that do not belong to any cone $\mathcal{K}_n^{(r)}$, disproving a conjecture from Dickinson et al. [7]. However, it is not known whether any 6×6 copositive matrix with an all-ones diagonal lies in the cone $\mathcal{K}_6^{(r)}$ for some $r \geq 1$.

We consider in detail the class of copositive matrices of the form $M_G = \alpha(G)(I + A_G) - J$, motivated by the stable set problem in a graph G . These matrices are recently investigated in the work Dickinson and de Zeeuw [6]. There, the question is to understand when the matrix M_G is irreducible with respect to the cone $\mathcal{K}_n^{(0)}$, which means that M_G cannot be written as $M_G = X + Y$ with $X \in \mathcal{K}_n^{(0)}$, $Y \in \text{COP}_n$ and $X, Y \neq 0$. This irreducibility property is

indeed a necessary condition for M_G to lie on an extreme ray of COP_n . It is shown in Dickinson and de Zeeuw [6] that M_G is irreducible with respect to $\mathcal{K}_n^{(0)}$ if and only if G is connected, critical, and α -covered, and the latter means that any two vertices that are not adjacent in G belong to a maximum stable set of G . The authors in Dickinson and de Zeeuw [6] also provide a multitude of new extreme rays of COP_n for $n \leq 13$ arising from these graph matrices.

Whether the graph matrix M_G belongs to the cone $\mathcal{K}_n^{(r)}$ for $r = \alpha(G) - 1$ (for some $r \geq 0$) is the object of Conjecture 1 posed in de Klerk and Pasechnik [4] (conjecture 2 posed in Laurent and Vargas [19]). The smallest r for which $M_G \in \mathcal{K}_n^{(r)}$ is $\vartheta\text{-rank}(G)$. So these two conjectures claim, respectively, that, for any graph G , $\vartheta\text{-rank}(G) \leq \alpha(G) - 1$ and $\vartheta\text{-rank}(G) < \infty$. The behavior of the ϑ -rank under the graph operation of adding an isolated node plays a crucial role in understanding these two conjectures. It is proved in Gvozdenović and Laurent [12] that Conjecture 1 holds if adding an isolated node does not increase the ϑ -rank. In this work, we show that adding an isolated node may increase the ϑ -rank, which disproves a conjecture from Gvozdenović and Laurent [12]. Namely, we show that C_5 together with eight isolated nodes has ϑ -rank one, whereas C_5 with nine isolated nodes has ϑ -rank at least two. This indicates that the full resolution of Conjecture 1 likely necessitates a novel idea. On the other hand, we show that Conjecture 2 holds if and only if adding an isolated node preserves finiteness of the ϑ -rank. This, thus, opens a possible direction to attack the (weaker) Conjecture 2. Recall that we show recently in Laurent and Vargas [19] that Conjecture 2 holds for the class of acritical graphs.

Finally, we characterize the critical graphs G with $\vartheta\text{-rank}(G) = 0$, and we investigate the graphs G for which $M_G \in \mathcal{K}_n^{(0)}$ from an algorithmic point of view. We show a reduction of this question to the class of acritical graphs. It is interesting to note that the “criticality” property plays a key role in understanding membership of the graph matrices M_G in the cones $\mathcal{K}_n^{(r)}$ as well as in the characterization of the irreducibility property in Dickinson and de Zeeuw [6].

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