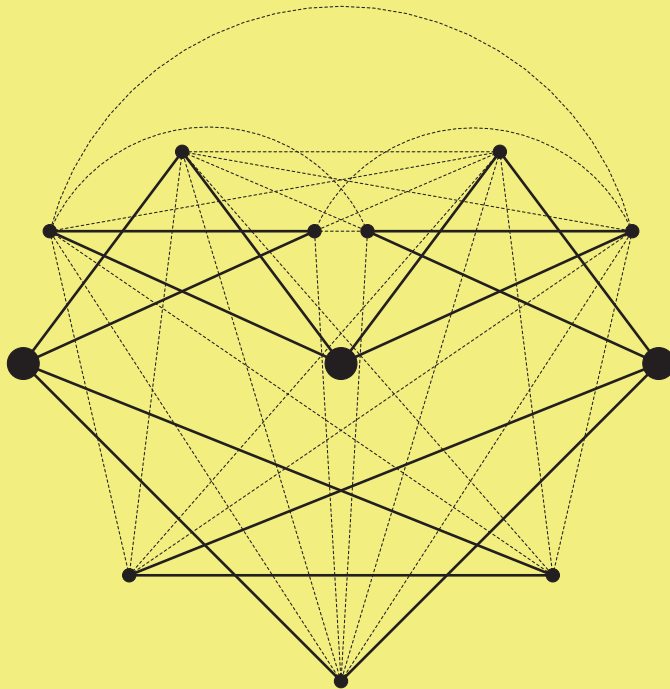




# Sum-of-Squares Representations for Copositive Matrices and Independent Sets in Graphs

LUIS FELIPE VARGAS BELTRÁN





# Sum-of-Squares Representations for Copositive Matrices and Independent Sets in Graphs

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**Luis Felipe Vargas Beltrán,**

geboren te Barrancabermeja, Colombia

PROMOTOR: prof. dr. M. Laurent (Tilburg University)

COPROMOTOR: dr. J.C. Vera Lizcano (Tilburg University)

PROMOTIECOMMISSIE: prof. dr. G. Blekherman (Georgia Institute of Technology)  
prof. dr. M. Dür (Augsburg University)  
prof. dr. E. de Klerk (Tilburg University)  
prof. dr. D.C. Gijswijt (TU Delft)  
prof. dr. F. Vallentin (University of Cologne)  
prof. dr. L.F. Zuluaga (Lehigh University)

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# Contents

Introduction .....	1
Sums of squares of polynomials and polynomial optimization .....	1
Copositive matrices .....	3
Certificates for copositivity using sums of squares .....	3
The stability number of a graph .....	5
Bicliques and biindependent pairs in bipartite graphs .....	6
Societal and scientific relevance .....	6
Organization .....	7
Publications .....	8
 Chapter 1. The copositive cone and sums of squares of polynomials .....	 11
1.1. The copositive cone .....	11
1.2. Polynomial optimization .....	11
1.3. Sum-of-squares certificates for nonnegativity .....	12
1.4. Semidefinite programming and sums of squares .....	16
1.5. Approximation hierarchies for polynomial optimization .....	17
1.6. Sum-of-squares approximations for $\text{COP}_n$ .....	20
 Chapter 2. Exactness of sum-of-squares approximations for $\text{COP}_n$ .....	 23
2.1. Constructing copositive matrices outside $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ .....	26
2.2. Links between the approximation cones for $\overline{\text{COP}}_n$ .....	27
2.3. Characterizing the equality $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} = \text{COP}_n$ .....	31
2.4. Main result .....	33
 Chapter 3. Semidefinite approximations for the stability number .....	 39
3.1. Lovász $\vartheta$ -number .....	39
3.2. Polynomial optimization formulations .....	40
3.3. Copositive formulation .....	42
3.4. The hierarchy $\vartheta^{(r)}(G)$ .....	43
 Chapter 4. Simplex-based approximations for $\alpha(G)$ .....	 49
4.1. Introduction .....	49
4.2. Sum-of-squares hierarchies for standard quadratic programs .....	52
4.3. Minimizers of the (weighted) Motzkin-Straus formulation .....	56
4.4. Finite convergence and perturbed hierarchies .....	61
4.5. Complexity results .....	67

Chapter 5. Low order sum-of-squares bounds for the stability number ..	71
5.1. Preliminaries on the cones $\mathcal{K}_n^{(0)}$ and $\mathcal{K}_n^{(1)}$ .....	73
5.2. $\vartheta$ -rank, simple graph operations and some examples .....	78
5.3. Towards characterizing graphs with $\vartheta$ -rank 0 .....	85
5.4. On the impact of isolated nodes on the $\vartheta$ -rank .....	95
5.5. Bounds $\nu^{(r)}$ and some extreme graph classes .....	107
Chapter 6. Test states and membership in quadratic modules .....	113
6.1. Preliminaries .....	115
6.2. Test states and membership in quadratic modules .....	116
6.3. Positive diagonal scalings of the Horn matrix .....	120
6.4. The hierarchy $\vartheta^{(r)}(G)$ has finite convergence .....	121
Chapter 7. Bicliques and biindependent sets .....	125
7.1. Introduction .....	125
7.2. Complexity results .....	131
7.3. Semidefinite approximations for the parameters $g(G)$ and $h(G)$ .	136
7.4. Eigenvalue bounds for the parameters $g(G)$ and $h(G)$ .....	143
7.5. Examples .....	152
7.6. Lasserre bounds for the balanced parameters .....	156
Chapter 8. Concluding remarks .....	163
Copositive matrices and the cones $\mathcal{K}_n^{(r)}$ .....	163
Graph matrices $M_G$ , cones $\mathcal{K}_n^{(r)}$ , $\text{LAS}_{\Delta_n}^{(r)}$ and $\mathcal{Q}_n^{(r)}$ .....	164
Constructing nonnegative polynomials that are not sums of squares ...	165
Complexity questions about polynomial optimization .....	165
Parameters in bipartite graphs .....	166
Bibliography .....	169
List of symbols .....	177
Graph theory .....	177
Polynomials .....	177
Matrices .....	177
special sets .....	177
Special polynomials and matrices .....	178
Polynomial optimization and sums of squares .....	178



# Introduction

This thesis explores the connection between three main topics in real algebraic geometry, optimization, and graph theory. Specifically, we study relations between sums of squares and nonnegative polynomials with a focus on their applications to problems involving copositive matrices and graph parameters.

Many combinatorial problems, such as the stable set problem, are known to be hard. Specifically, assuming the well-believed conjecture claiming that  $P \neq NP$ , there is no efficient algorithm for solving such problems. A common approach for addressing this hardness issue is by considering variations of the original problem that give an approximate solution, and that can be computed efficiently. One of these approaches for attacking hard combinatorial problems and, more generally, polynomial optimization problems, is given by the so-called sum-of-squares hierarchies.

The interest for studying sums of squares of polynomials in the context of optimization has increased in the last decades thanks to the following crucial fact: A polynomial  $p \in \mathbb{R}[x]$  of degree  $2d$  is a sum of squares if and only if there exists a positive semidefinite matrix  $Q$  such that

$$p(x) = [x]_d^\top Q [x]_d,$$

where  $[x]_d = (x_1, \dots, x_n, x_1x_2, \dots, x_n^d)^\top$  is the vector of monomials of degree at most  $d$ . Then, optimization problems that involve constraints asking for the existence of a decomposition using sums of squares can be modeled by a *semi-definite program*. This key observation motivates to study approximations for hard problems using sums of squares. This is the starting point for defining the so-called sum-of-squares hierarchies for polynomial optimization, as shown by Lasserre [Las01b]. In addition, as we will see, sums of squares of polynomials also provide tractable approximations for copositive programming, as first shown by Parrilo [Par00].

## Sums of squares of polynomials and polynomial optimization

Given a multivariate polynomial  $p \in \mathbb{R}[x]$ , the problem of determining whether  $p$  is nonnegative, i.e.,  $p(x) \geq 0$  for all  $x \in \mathbb{R}^n$ , is a well-known hard problem. A first try for showing that the polynomial  $p$  is nonnegative is by

looking for a decomposition as a sum of squares. A polynomial  $p \in \mathbb{R}[x]$  is called a *sum of squares* if

$$p = q_1^2 + q_2^2 + \cdots + q_m^2$$

for some other polynomials  $q_1, \dots, q_m \in \mathbb{R}[x]$ . Clearly, if  $p$  is a sum of squares, then  $p$  is globally nonnegative. The connection between nonnegative polynomials and sums of squares has been studied in depth in the last centuries. In 1888, Hilbert [**Hilb88**] showed that there exist nonnegative polynomials that cannot be written as a sum of squares. Moreover, he characterized the degrees and dimensions for which every nonnegative polynomial can be written as a sum of squares. Later in 1927, Artin [**Art27**] showed that every nonnegative polynomial can be written as a sum of squares of ratios of polynomials, solving affirmatively Hilbert’s 17-th problem. This last result by Artin shows that it is indeed possible to prove that a polynomial is nonnegative by using sums of squares of polynomials in a certain way. Later, the results by Pólya [**Poly28**] and Reznick [**Rez95**] show the existence of such certificates in a more structured form for homogenous polynomials that satisfy a strict positivity condition.

The question of determining whether a polynomial  $p$  is nonnegative over a basic closed semialgebraic set  $K$  (i.e., described by finitely many polynomial inequalities) has also been studied. The results by Schmüdgen [**Schm91**] and Putinar [**Put93**] showing the existence of sum-of-squares certificates for  $p$  on  $K$  (under some technical assumptions) have been the basis for constructing tractable approximations for polynomial optimization problems, as described by Lasserre [**Las01a**] and Parrilo [**Par00**].

A polynomial optimization problem asks for minimizing a polynomial function  $f \in \mathbb{R}[x]$  over a set defined by polynomial inequalities ( $g_i(x) \geq 0$  for  $i = 1, \dots, m$ ) and polynomial equations ( $h_j(x) = 0$  for  $j = 1, \dots, l$ ). Thus, it reads

$$\min_{x \in K} f(x), \quad \text{where } K = \left\{ x \in \mathbb{R}^n : g_i(x) \geq 0 \text{ for } i \in [m], h_j(x) = 0 \text{ for } j \in [l] \right\}.$$

Polynomial optimization permits to model many hard problems. Since the constraint “ $x_i = 0$  or  $x_i = 1$ ” can be modeled by the polynomial equation  $x_i^2 - x_i = 0$ , many hard combinatorial problems, such as the stability number of a graph or MAX-CUT, can be naturally encoded as polynomial optimization problems and the machinery of sums of squares approximations can be applied. Other instances of polynomial optimization, such as linear and quadratic optimization over the standard simplex  $\Delta_n$ , or optimization over the unit sphere  $\mathbb{S}^{n-1}$ , have been shown to have many applications in portfolio optimization, energy optimization, and combinatorial optimization. See, for example, [**Las09**].

## Copositive matrices

A main object of study in this thesis is the cone of copositive matrices, known as the *copositive cone*. An  $n \times n$  symmetric matrix  $M$  is said to be *copositive* if the associated quadratic form  $x^T M x = \sum_{i,j=1}^n M_{ij} x_i x_j$  is non-negative over the nonnegative orthant  $\mathbb{R}_+^n$ . The set of copositive matrices is a cone, the *copositive cone*  $\text{COP}_n$ , thus defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : x^T M x \geq 0 \quad \forall x \in \mathbb{R}_+^n\}.$$

Copositive matrices were first introduced by Motzkin [Mot52] in 1952 and they have been an active research topic since then. Some of the topics that have been studied are: methods for determining copositivity [CHL70], description of the extreme rays of  $\text{COP}_n$  ([Hil12, HA22]), copositive completion problems [HJR05] and optimization [BdK02].

The connection between the copositive cone and optimization received great attention since 2000, when Bomze et al. [BDdKRQT00] established a formulation of an NP-hard problem as a linear optimization over  $\text{COP}_n$  and introduced the term *copositive programming*. Since then, many combinatorial problems, including the stability and chromatic number of a graph, have been formulated as copositive programs. We refer to the survey [Dür10] for more examples and applications. Later, in 2009, Burer [Bu09] showed a much more general result: every quadratic program including continuous and binary variables can be encoded as a copositive program. As expected, optimizing over  $\text{COP}_n$  is hard. Moreover, the problem of determining whether a matrix is copositive is a co-NP-complete problem [MK87]. These results motivate to study tractable approximations for copositive programs and certificates for copositivity.

The copositive cone can be equivalently defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \geq 0 \quad \forall x \in \mathbb{R}^n\}, \quad (0.1)$$

where we set  $x^{\circ 2} = (x_1^2, \dots, x_n^2)$ . Hence, determining whether a matrix  $M$  is copositive is equivalent to determine whether the quartic form

$$(x^{\circ 2})^T M x^{\circ 2}$$

is globally nonnegative. A main topic in this thesis is a study of certificates for copositivity using sums of squares of polynomials.

## Certificates for copositivity using sums of squares

As mentioned before, determining whether a matrix  $M$  is copositive amounts to determine whether the associated polynomial  $(x^{\circ 2})^T M x^{\circ 2}$  is non-negative. It was shown (see [Dian62, Par00]) that, for every  $n \times n$  copositive matrix  $M$  with  $n \leq 4$ , the polynomial  $(x^{\circ 2})^T M x^{\circ 2}$  is a sum of squares. This result does not extend to  $n \geq 5$ . Nevertheless, there are two alternative recipes

for certifying that a matrix is copositive by using sums of squares. First, if for some  $r \in \mathbb{N}$ , the polynomial

$$\left( \sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^\top M x^{\circ 2} \quad \text{is a sum of squares,} \quad (0.2)$$

then  $M$  is copositive. This certificate was proposed by Parrilo in [Par00] and it is based on the certificates for nonnegative polynomials by Pólya [Poly28] and Reznick [Rez95]. It is shown that every matrix in the interior of the copositive cone admits a certificate as in (0.2). A central topic in this thesis is an intensive study for understanding whether this certificate exists for matrices in the *boundary* of the copositive cone. These certificates were used by Parrilo for optimization purposes [Par00], and later used by de Klerk and Pasechnik [dKP02] who defined the following cones  $\mathcal{K}_n^{(r)} \subseteq \text{COP}_n$  for approximating the stability number of a graph:

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^\top M x^{\circ 2} \text{ is a sum of squares} \right\}.$$

The key point is that, while linear optimization over  $\text{COP}_n$  is hard, optimizing a linear function over  $\mathcal{K}_n^{(r)}$  can be done via semidefinite programming. Thus, the cones  $\mathcal{K}_n^{(r)}$  give tractable approximations for linear optimization problems over  $\text{COP}_n$ .

Alternatively, if there exist sums of squares  $\sigma_0, \sigma_1, \dots, \sigma_n$  and  $q \in \mathbb{R}[x]$  such that

$$x^\top M x = \sigma_0 + x_1 \sigma_1 + \dots + \sigma_n x_n + q \left( \sum_{i=1}^n x_i - 1 \right), \quad (0.3)$$

then the matrix  $M$  is copositive. This certificate is based on Putinar's Positivstellensatz [Put93] and the Lasserre sum-of-squares hierarchy for polynomial optimization [Las01a]. Similarly, every matrix in the interior of the copositive cone admits a certificate as in (0.3). In addition, we will show that every matrix satisfying a certificate as in (0.3) also admits a certificate as in (0.2). We consider several other certificates for copositivity (e.g., the ones using the cones  $\mathcal{Q}_n^{(r)}$  proposed by de Peña, Vera and Zuluaga in [PVZ07], or the ones using the cones  $\mathcal{C}_n^{(r)}$  proposed by de Klerk and Pasechnik in [dKP02]). We study in detail properties that permit to show the existence of these certificates.

One of the main results of this thesis is a full characterization of the matrix sizes for which every copositive matrix admits a certificate as in (0.2). In other words, we characterize the matrix sizes  $n$  for which the cones  $\mathcal{K}_n^{(r)}$  cover the full

copositive cone  $\text{COP}_n$ . The proof of this result has two main technical steps that require different techniques, as we will show in Chapter 2 and Chapter 6.

### The stability number of a graph

Given a graph  $G = (V, E)$ , a subset of vertices  $S \subseteq V$  is *stable* (or *independent*) if  $S$  contains no edge, i.e.,  $\{i, j\} \notin E$  for any  $i, j \in S$ . The stability number of  $G$ , denoted by  $\alpha(G)$ , is the maximum cardinality of a *stable* set in  $G$ . Computing  $\alpha(G)$  is a central problem in combinatorial optimization, well-known to be NP-hard, with many applications in various areas, such as scheduling, social networks analysis, and bioinformatics (see, e.g., [BBPP99], [WH15]). Several approaches for approximating  $\alpha(G)$  have been proposed, including the use of semidefinite programming. The best-known bound for  $\alpha(G)$  is the Lovász-theta number  $\vartheta(G)$ , defined by Lovász [Lov79] in his seminal paper in 1979, with the purpose of computing the Shannon capacity of graphs. De Klerk and Pasechnik [dKP02] established a formulation of  $\alpha(G)$  as a copositive program:

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

From this formulation, we obtain that for every graph  $G$  the matrix

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

is copositive. This class of copositive matrices offers a very rich playground for analyzing properties of the copositivity certificates as well as complexity aspects of polynomial optimization problems, as will see in Chapters 4, 5 and 6.

De Klerk and Pasechnik [dKP02] used the cones  $\mathcal{K}_n^{(r)}$  for defining a hierarchy of upper bounds for  $\alpha(G)$  that strengthen the bound given by the Lovász-theta number  $\vartheta(G)$ :

$$\vartheta^{(r)}(G) := \min \left\{ t : t(A_G + I) - J \in \mathcal{K}_n^{(r)} \right\}.$$

These bounds are shown to converge asymptotically to  $\alpha(G)$  as  $r \rightarrow \infty$ . It was conjectured in [dKP02] that finite convergence takes place after  $\alpha(G) - 1$  steps. In this thesis, we study the parameters  $\vartheta^{(r)}(G)$  in detail. As a main result, we obtain the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  to  $\alpha(G)$ . The proof of this result consists of two main steps. First, in Chapter 5, we show that the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence for every graph if and only if the finite convergence of  $\vartheta^{(r)}(G)$  is preserved after the simple graph operation of adding an isolated node. Then, in Chapter 6, we show that this last property holds for every graph. For this, we develop an algebraic tool for showing membership in quadratic modules.

We study situations in which the low level approximations  $\vartheta^{(r)}(G)$  ( $r = 0, 1$ ) are exact and show that the graph structure (e.g., critical edges and

isolated nodes) plays a crucial role in this analysis. We also study the analogous bounds obtained by using other sum-of-squares certificates for copositivity and we analyze the behavior and exactness of these bounds. This a central topic in Chapters 4 and 5.

### Bicliques and biindependent pairs in bipartite graphs

Let  $G = (V_1 \cup V_2, E)$  be a bipartite graph. A pair  $(A, B)$  with  $A \subseteq V_1$ ,  $B \subseteq V_2$  is *biindependent* if  $A \cup B$  is independent (or stable) in  $G$ . In this thesis, we study the parameters  $g(G)$  and  $h(G)$  defined, respectively, as the maximum product  $|A| \cdot |B|$ , and the maximum ratio  $|A| \cdot |B|/|A \cup B|$  taken over all biindependent pairs  $(A, B)$  in  $G$ . Thus,

$$g(G) := \max\{|A| \cdot |B| : (A, B) \text{ is a bipartite biindependent pair in } G\},$$

$$h(G) := \max\left\{\frac{|A| \cdot |B|}{|A| + |B|} : (A, B) \text{ is a bipartite biindependent pair in } G\right\}.$$

The parameter  $g(\cdot)$  is NP-hard to compute [Pe03]. This parameter permits to model maximum edge cardinality bicliques in bipartite (or general) graphs [DKT97, ST98] and has many applications such as reducing assembly times in product manufacturing lines [DKST01]. We show that the parameter  $h(\cdot)$  is also NP-hard to compute. This parameter was first introduced by Vallentin [Val20] who observed its relevance to maximum product-free subsets in groups. The related parameter  $\alpha_{\text{bal}}(G)$  asking for the maximum of  $|A| + |B|$  taken over *balanced biindependent sets* (e.g.,  $(A, B)$  biindependent with  $|A| = |B|$ ) is also considered in this thesis. We show that computing  $\alpha_{\text{bal}}(G)$  is NP-hard. This parameter has applications in VLSI design (e.g., [AYRP07, RL88, Tah06]), and in the analysis of biological data.

The hardness results for the parameters  $g(\cdot)$  and  $h(\cdot)$  motivate to study tractable approximations for them. We formulate  $g(\cdot)$  and  $h(\cdot)$  as polynomial optimization problems and consider their corresponding Lasserre sum-of-squares hierarchies. In particular, we study the first level bounds obtained from both hierarchies and we observe that they can be seen as quadratic variations of the Lovász-theta number. In addition, we give closed-form eigenvalue bounds for the parameters  $h(\cdot)$  and  $g(\cdot)$ , and we show relationships with earlier spectral parameters by Hoffman [Haem21], Haemers [Haem01], and Vallentin [Val20]. We also investigate semidefinite bounds for the balanced parameter  $\alpha_{\text{bal}}(G)$  and their links to the theta number.

### Societal and scientific relevance

In this thesis, we study tractable approximations using sum-of-squares polynomials in two general settings: for approximating the copositive cone and for approximating graph parameters such as the stability number of a graph and parameters in bipartite graphs. Copositive programming permits

to model any quadratic program with binary variables. Then, a broad class of real-life problems can be modeled as copositive programs. Some of the remarkable applications are in dynamical systems and optimal control (e.g., [QDM92]), modeling friction, and contact problems in body rigid mechanics (e.g., [ACP97, AP02]) and in network problems such as in queueing, traffic, and reliability (e.g., [KM96, MK99]). Our results give a comparison between several different approaches for copositive programming based on sums of squares of polynomials.

The problem of computing the stability number of a graph (and the related problem of finding the maximum clique) has many applications in different areas, among others, in scheduling, social networks analysis and bioinformatics (see [BBPP99], [WH15]). In this thesis we also study parameters in bipartite graphs that, as mentioned earlier, have applications in product manufacturing, VLSI design [AYRP07, RL88, Tah06], in the analysis of biological data [YWWY05] and in the analysis of interactions of proteins [MRU87]).

## Organization

The thesis is organized as follows. In Chapter 1, we introduce the general background of positive polynomials, sums of squares and polynomial optimization. We also describe several conic approximations for the copositive cone  $\text{COP}_n$  based on sums of squares of polynomials, that will be studied throughout in different contexts in the rest of the thesis.

In Chapter 2, we study the question of whether the conic approximations for  $\text{COP}_n$  defined in Chapter 1 are exact. In other words, we study situations in which some sum-of-squares certificates for matrix copositivity exist. For this, we show links between the various approximation cones and we study the exactness of each of them independently. In particular, we give special attention to the cone of  $5 \times 5$  copositive matrices that, as we will show, is arguably the most interesting case to study.

In Chapter 3, we introduce some classical semidefinite bounds for the stability number  $\alpha(G)$ , including the Lovász theta number. We also recall the formulation of  $\alpha(G)$  as a copositive program and some hierarchies of approximations for  $\alpha(G)$  defined in the literature. In particular, we recall the bounds  $\vartheta^{(r)}(G)$  and summarize the main known results about this hierarchy.

In Chapter 4, we consider the Motzkin-Straus formulation, a well-known formulation for  $\alpha(G)$  as a standard quadratic program, and its corresponding Lasserre sum-of-squares hierarchy. We characterize the graphs for which their corresponding Lasserre hierarchy has finite convergence. As an application, we obtain two complexity results about polynomial optimization problems and

their corresponding Lasserre sum-of-squares hierarchies.

In Chapter 5, we study the low order bounds  $\vartheta^{(0)}(G)$  and  $\vartheta^{(1)}(G)$  and show how some simple graph operations play a crucial role in their analysis. We also show that the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence for every graph  $G$  if and only if the finite convergence of  $\vartheta^{(r)}(G)$  is preserved after adding isolated nodes. This result will be used in Chapter 6 for showing the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ . In addition, we develop a tool for showing that certain copositive matrices arising from graphs require a high degree sum-of-squares certificate.

In Chapter 6, we develop an algebraic tool for showing membership in quadratic modules. As a main application, we show the existence of certificates for copositivity for two classes of copositive matrices: the  $5 \times 5$  copositive matrices and the graph matrices  $M_G$ . This permits to show two main results of this thesis: Namely,  $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ , and the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence to  $\alpha(G)$  for every graph  $G$ .

In Chapter 7, we study several parameters in bipartite graphs. We show that these parameters are NP-hard to compute and we propose semidefinite formulation to approximate them, as well as closed-form eigenvalue bounds.

Finally, in Chapter 8, we briefly summarize the main results of the thesis and we highlight some open questions and possible directions for future research.

## Publications

This thesis is based on the following three published papers, a book chapter, a preprint, and a work in preparation:

- [LV22a] M. Laurent, L.F. Vargas, Finite convergence of sum-of-squares hierarchies for the stability number of a graph. *SIAM Journal on Optimization*, 32(2):491-518, 2022.
- [LV22b] M. Laurent, L.F. Vargas, Exactness of Parrilo's conic approximations for copositive matrices and associated low order bounds for the stability number of a graph. *Mathematics of Operations Research*, 48(2): 1017-1043, 2022.
- [LV22c] M. Laurent, L.F. Vargas, On the exactness of sum-of-squares approximations for the cone of  $5 \times 5$  copositive matrices. *Linear Algebra and its Applications*, 651:26–50, 2022.
- [VL23] L.F. Vargas, M. Laurent. Copositive matrices, sums of squares and the stability number of a graph. Michal Kočvara, Bernard Mourrain, Cordian Riener (eds.). In: *Polynomial Optimization, Moments, and Applications*, Springer, pp. 99-132, in press.



- [LPV23] M. Laurent, S. Polak, L.F. Vargas. Semidefinite approximations for bicliques and biindependent pairs. Preprint, arXiv:2302.08886, 2023.
- [SV23] M. Schweighofer, L.F. Vargas. Sum-of-squares representations for copositive matrices and the stability number of a graph. In preparation, 2023+.



# The copositive cone and sums of squares of polynomials

## 1.1. The copositive cone

An  $n \times n$  symmetric matrix  $M$  is said to be *copositive* if the associated quadratic form  $x^T M x = \sum_{i,j=1}^n M_{ij} x_i x_j$  is nonnegative over the nonnegative orthant  $\mathbb{R}_+^n$ . The set of copositive matrices is a cone, the *copositive cone*  $\text{COP}_n$ , thus defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : x^T M x \geq 0 \quad \forall x \in \mathbb{R}_+^n\}. \quad (1.1)$$

Equivalently, the copositive cone is defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \geq 0 \quad \forall x \in \mathbb{R}^n\}, \quad (1.2)$$

where we let  $x^{\circ 2} = (x_1^2, \dots, x_n^2)$ . Hence, determining whether a matrix  $M$  is copositive amounts to determine whether the quartic form

$$(x^{\circ 2})^T M x^{\circ 2}$$

is globally nonnegative. As mentioned in the Introduction, optimizing over  $\text{COP}_n$  is hard as many hard problems, including the stability and chromatic number of a graph, can be encoded as a linear optimization problem over  $\text{COP}_n$ . Moreover, the problem of determining whether a matrix is copositive is a co-NP-complete problem [MK87]. Motivated by these hardness results, some conic semidefinite approximations for the copositive cone have been proposed. In particular, some of them are based on using sums of squares of polynomials. In this chapter, we recall the general background of polynomial optimization. In particular, we recall several results for certifying the nonnegativity of a polynomial by using sums of squares of polynomials. These results are used for building tractable approximations for polynomial optimization problems. Moreover, these certificates also permit to build inner conic approximations for  $\text{COP}_n$ , as described in Section 1.6.

## 1.2. Polynomial optimization

Polynomial optimization asks for minimizing a polynomial over a semi-algebraic set. That is, given polynomials  $f, g_1, \dots, g_m, h_1, \dots, h_l \in \mathbb{R}[x]$ , the

task is to find (or approximate) the infimum of the following problem:

$$f^* = \inf_{x \in K} f(x), \quad (1.3)$$

where

$$K = \left\{ x \in \mathbb{R}^n : g_i(x) \geq 0 \text{ for } i = 1, \dots, m \text{ and } h_i(x) = 0 \text{ for } i = 1, \dots, l \right\} \quad (1.4)$$

is a semialgebraic set. Problem (1.3) can be equivalently rewritten as

$$f^* = \sup\{\lambda : f(x) - \lambda \geq 0 \text{ for all } x \in K\}. \quad (1.5)$$

In view of this new formulation, finding lower bounds for a polynomial optimization problem amounts to finding certificates that certain polynomials are nonnegative on the semialgebraic set  $K$ .

### 1.3. Sum-of-squares certificates for nonnegativity

Testing whether a polynomial is nonnegative on a semialgebraic set is hard in general. Even testing whether a polynomial is globally nonnegative (nonnegative on  $K = \mathbb{R}^n$ ) is a hard task in general. An easy *sufficient* condition for a polynomial to be globally nonnegative is being a sum of squares. A polynomial  $p \in \mathbb{R}[x]$  is said to be a *sum of squares* if it can be written as a sum of squares of other polynomials, i.e., if  $p = q_1^2 + \dots + q_m^2$  for some  $q_1, \dots, q_m \in \mathbb{R}[x]$ . We denote by  $\Sigma$  the set of sums of squares of polynomials and set  $\Sigma_r = \Sigma \cap \mathbb{R}[x]_r$ , where  $\mathbb{R}[x]_r$  denotes the set of polynomials of degree at most  $r$ . Hilbert [**Hilb88**, **Hilb93**] showed that every nonnegative polynomial of degree  $2d$  in  $n$  variables is a sum of squares in the following cases:  $(2d, n) = (2d, 1)$ ,  $(2, n)$ , or  $(4, 2)$ . Moreover, he showed that for any other pair  $(2d, n)$  there exist nonnegative polynomials that are not sums of squares. The first explicit example of a nonnegative polynomial that is not a sum of squares was given by Motzkin [**Mot67**] in 1967.

**Example 1.1.** *The following polynomial in two variables is known as the Motzkin polynomial:*

$$h(x, y) = x^4y^2 + x^2y^4 - 3x^2y^2 + 1. \quad (1.6)$$

*The Motzkin polynomial is nonnegative on  $\mathbb{R}^2$ . This can be seen, e.g., by using the Arithmetic-Geometric Mean inequality, which gives*

$$\frac{x^4y^2 + x^2y^4 + 1}{3} \geq \sqrt[3]{x^4y^2 \cdot x^2y^4 \cdot 1} = x^2y^2.$$

*However,  $h(x, y)$  cannot be written as a sum of squares. This can be checked using “brute force”: assume  $h = \sum_i q_i^2$  and examine the coefficients on both sides (starting from the coefficients of the monomials  $x^6, y^6$ , etc.; see, e.g., [**Rez00**]).*

The Motzkin form is the homogenization of  $h$ , thus the homogeneous polynomial in three variables:

$$m(x, y, z) = x^4y^2 + x^2y^4 - 3x^2y^2z^2 + z^6. \quad (1.7)$$

Hence, the Motzkin form is nonnegative on  $\mathbb{R}^3$  and it cannot be written as a sum of squares.

In 1927, Artin [Art27] proved that any globally nonnegative polynomial  $f$  can be written as a sum of squares of rational functions, i.e.,  $f = \sum_i (\frac{p_i}{q_i})^2$  for some  $p_i, q_i \in \mathbb{R}[x]$ , solving affirmatively Hilbert's 17th problem. Equivalently, Artin's result shows that for any nonnegative polynomial  $f$  there exists a polynomial  $q$  such that  $q^2f \in \Sigma$ . The following result shows that, when  $f$  is homogeneous and strictly positive on  $\mathbb{R}^n \setminus \{0\}$ , the multiplier  $q^2$  can be chosen to be a power of  $(\sum_{i=1}^n x_i^2)$ .

**Theorem 1.2** (Reznick [Rez95]). *Let  $f \in \mathbb{R}[x]$  be a homogeneous polynomial such that  $f(x) > 0$  for all  $x \in \mathbb{R}^n \setminus \{0\}$ . Then the following holds:*

$$\left( \sum_{i=1}^n x_i^2 \right)^r f \in \Sigma \quad \text{for some } r \in \mathbb{N}. \quad (1.8)$$

Scheiderer [Sche06] shows that the *strict* positivity condition can be omitted for  $n = 3$ : any *nonnegative* form  $f$  in three variables admits a certificate as in (1.8). On the negative side, this is not the case for  $n \geq 4$ : there exist nonnegative forms in  $n \geq 4$  variables that do not admit a positivity certificate as in (1.8). An example is given in Example 1.4.

**Example 1.3.** *Let  $h(x, y) = x^4y^2 + x^2y^4 - 3x^2y^2 + 1$  be the Motzkin polynomial, which is nonnegative and not a sum of squares. However,*

$$(x^2 + y^2)^2 h(x, y) = x^2y^2(x^2 + y^2 + 1)(x^2 + y^2 - 2)^2 + (x^2 - y^2)^2$$

*is a sum of squares. This sum-of-squares certificate thus shows (again) that  $h$  is nonnegative on  $\mathbb{R}^2$ .*

**Example 1.4.** *Let  $q(x, y, z, w) := m(x, y, z)^2 + w^6m(x, y, z)$ , where  $m(x, y, z)$  is the Motzkin form from (1.7). Clearly,  $q$  is nonnegative on  $\mathbb{R}^4$ , as  $m$  is nonnegative on  $\mathbb{R}^3$ . Assume that the polynomial  $(x^2 + y^2 + z^2 + w^2)^r q$  is a sum of squares for some  $r \in \mathbb{N}$ . Then,*

$$q' := (x^2 + y^2 + z^2 + 1)^r q(x, y, z, 1) = (x^2 + y^2 + z^2 + 1)^r (m^2 + m)$$

*is also a sum of squares. As  $q'$  is a sum of squares, one can check that also its lowest degree homogeneous part is a sum of squares (see Chapter 2, Lemma 2.6). However, the lowest degree homogeneous part of  $q'$  is  $m$ , which is not a sum of squares. Hence this shows that  $(x^2 + y^2 + z^2 + w^2)^r q \notin \Sigma$  for all  $r \in \mathbb{N}$ .*

Next, we give some positivity certificates for polynomials on semialgebraic sets. The following result shows the existence of a positivity certificate for polynomials that are strictly positive on the nonnegative orthant  $\mathbb{R}_+^n$ .

**Theorem 1.5** (Pólya [Poly28]). *Let  $f$  be a homogeneous polynomial such that  $f(x) > 0$  for all  $x \in \mathbb{R}_+^n \setminus \{0\}$ . Then the following holds:*

$$\left( \sum_{i=1}^n x_i \right)^r f \text{ has nonnegative coefficients for some } r \in \mathbb{N}. \quad (1.9)$$

In addition, Castle, Powers, and Reznick [CPR09] show that nonnegative polynomials on  $\mathbb{R}_+^n$  with simple zeros also admit a certificate as in (1.9). Given a homogeneous polynomial  $p \in \mathbb{R}[x]$  of degree  $d$ , a *simple zero* of  $p$  is a zero of the form  $x = e_i$  ( $i \in [n]$ ), where the coefficient of  $x_i^d$  in  $p$  is zero, and the coefficient of  $x_i^{d-1}x_j$  is positive for all  $j \neq i$ .

**Theorem 1.6** ([CPR09]). *Let  $p \in \mathbb{R}[x]$  be a homogeneous polynomial. Assume  $p$  is nonnegative on  $\Delta_n$ , and  $p$  only has simple zeros in  $\Delta_n$ . Then,  $p$  admits a certificate as in (1.9).*

Now we consider positivity certificates for polynomials restricted to compact semialgebraic sets. Let  $\mathbf{g} = \{g_1, \dots, g_m\}$  and  $\mathbf{h} = \{h_1, \dots, h_l\}$  be sets of polynomials and consider the semialgebraic set  $K$  defined as in (1.4). The *quadratic module* generated by  $\mathbf{g}$ , denoted by  $\mathcal{M}(\mathbf{g})$ , is defined as

$$\mathcal{M}(\mathbf{g}) := \left\{ \sum_{i=0}^m \sigma_i g_i : \sigma_i \in \Sigma \text{ for } i = 0, 1, \dots, m, \text{ and } g_0 := 1 \right\}, \quad (1.10)$$

and the *preordering* generated by  $\mathbf{g}$ , denoted by  $\mathcal{T}(\mathbf{g})$ , is defined as

$$\mathcal{T}(\mathbf{g}) := \left\{ \sum_{J \subseteq [m]} \sigma_J \prod_{i \in J} g_i : \sigma_J \in \Sigma \text{ for } J \subseteq \{1, \dots, m\}, \text{ and } g_\emptyset := 1 \right\}. \quad (1.11)$$

The ideal generated by the polynomial set  $\mathbf{h}$  is defined as

$$I(\mathbf{h}) := \left\{ \sum_{i=1}^l p_i h_i : p_i \in \mathbb{R}[x] \text{ for } i \in [l] \right\}.$$

Observe that, if for a polynomial  $f$  we have

$$f \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h}), \quad (1.12)$$

$$\text{or } f \in \mathcal{T}(\mathbf{g}) + I(\mathbf{h}), \quad (1.13)$$

then  $f$  is nonnegative on  $K$ . Moreover, if a polynomial admits a certificate as in (1.12), then it also admits a certificate as in (1.13), because  $\mathcal{M}(\mathbf{g}) \subseteq \mathcal{T}(\mathbf{g})$ . We will refer to the quadratic module and preordering associated to the set

$$\mathbf{x} = \{x_1, \dots, x_n\}$$

as follows:

$$\mathcal{M}(\mathbf{x}) := \mathcal{M}(\{x_1, \dots, x_n\}) \quad \mathcal{T}(\mathbf{x}) := \mathcal{T}(\{x_1, \dots, x_n\}). \quad (1.14)$$

Also, we refer to the ideal generated by the polynomials  $\sum_{i=1}^n x_i - 1$  and  $\sum_{i=1}^n x_i^2 - 1$ , respectively, as the simplex and sphere ideal and we write

$$I_{\Delta_n} := I\left(\sum_{i=1}^n x_i - 1\right) \quad \text{and} \quad I_{\mathbb{S}^{n-1}} := I\left(\sum_{i=1}^n x_i^2 - 1\right).$$

**Example 1.7.** Consider the polynomial  $p(x, y) = x^2 + y^2 - xy$  in two variables  $x, y$ . We show that  $p$  is nonnegative on  $\mathbb{R}_+^2$  in two different ways. The following identities hold:

$$\begin{aligned} (x + y)p(x, y) &= x^3 + y^3, \\ p(x, y) &= (x - y)^2 + xy, \end{aligned}$$

which both certify that  $p$  is nonnegative on  $\mathbb{R}_+^2$ . The first identity is a certificate as in (1.9):  $x^3 + y^3$  has nonnegative coefficients. The second identity shows that  $p \in \mathcal{T}(\{x, y\})$ , i.e., gives a certificate as in (1.13).

The following two theorems show that under certain conditions on the semialgebraic set  $K$  (and on the sets  $\mathbf{g}$  and  $\mathbf{h}$  defining it), every strictly positive polynomial admits certificates as in (1.12) or (1.13).

**Theorem 1.8** (Schmüdgen [Schm91]). Let  $\mathbf{g} = \{g_1, g_2, \dots, g_m\}$  and  $\mathbf{h} = \{h_1, \dots, h_l\}$  be sets of polynomials. Assume the semialgebraic set  $K$  defined by  $\mathbf{g}$  and  $\mathbf{h}$  as in (1.4) is compact. Let  $f \in \mathbb{R}[x]$  such that  $f(x) > 0$  for all  $x \in K$ . Then we have  $f \in \mathcal{T}(\mathbf{g}) + I(\mathbf{h})$ .

We say that the sets of polynomials  $\mathbf{g} = \{g_1, \dots, g_m\}$  and  $\mathbf{h} = \{h_1, \dots, h_l\}$  satisfy the Archimedean condition if

$$N - \sum_{i=1}^n x_i^2 \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h}) \quad \text{for some } N \in \mathbb{N}. \quad (1.15)$$

Note this implies that the associated set  $K$  is compact. We have the following result.

**Theorem 1.9** (Putinar [Put93]). Assume that the sets of polynomials  $\mathbf{g} = \{g_1, \dots, g_m\}$  and  $\mathbf{h} = \{h_1, \dots, h_l\}$  satisfy the Archimedean condition (1.15). Let  $K$  be the semialgebraic set defined by the sets  $\mathbf{g}$  and  $\mathbf{h}$  as in (1.4). Let  $f \in \mathbb{R}[x]$  be such that  $f(x) > 0$  for all  $x \in K$ . Then we have  $f \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h})$ .

### 1.4. Semidefinite programming and sums of squares

In this section, we recall the relation between semidefinite programming and sums of squares of polynomials. A key point is that positive semidefinite matrices permit to model sums of squares of polynomials. A symmetric matrix  $M \in \mathcal{S}^n$  is said to be *positive semidefinite*, and we write  $M \succeq 0$ , if any of the following equivalent assertions holds:

- (i):  $x^\top Mx \geq 0$  for all  $x \in \mathbb{R}^n$ .
- (ii): The eigenvalues of  $M$  are nonnegative, i.e.,  $M = \sum_{i=1}^n \lambda_i u_i u_i^\top$  for some nonnegative scalars  $\lambda_i \in \mathbb{R}_+$  and orthonormal vectors  $u_i \in \mathbb{R}^n$  for  $i \in [n]$ .

We write  $A \succeq B$  if  $A - B \succeq 0$ . We say that a matrix is *positive definite*, and we write  $M \succ 0$ , if  $x^\top Mx > 0$  whenever  $x \neq 0$ . A useful result for testing whether a matrix is positive semidefinite is the following.

**Lemma 1.10** (Schur Complement). *Let  $X \in \mathcal{S}^n$  be a matrix in block form*

$$X = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix},$$

where  $A \in \mathcal{S}^m$ ,  $C \in \mathcal{S}^{n-m}$  and  $B \in \mathbb{R}^{m \times (n-m)}$ . If  $A$  is nonsingular, then

$$X \succeq 0 \iff A \succeq 0 \text{ and } C - B^\top A^{-1} B \succeq 0.$$

**1.4.1. Semidefinite programming.** Let  $C, A_1, \dots, A_m \in \mathcal{S}^n$  be symmetric matrices and let  $b_1, \dots, b_m \in \mathbb{R}$ . A program of the form

$$p^* = \sup \{ \langle C, X \rangle : \langle A_i, X \rangle = b_i \text{ for } i = 1, \dots, m, X \succeq 0 \} \quad (\text{P})$$

is called a *semidefinite program* (SDP). If the program (P) is not feasible we set  $p = -\infty$  and we set  $p = \infty$  if the program is unbounded. The associated *dual program* of (P) is the following:

$$d^* = \inf_{y \in \mathbb{R}^m} \left\{ \sum_{i=1}^m y_i b_i : \sum_{i=1}^m y_i A_i - C \succeq 0 \right\}. \quad (\text{D})$$

The programs (P) and (D) satisfy weak duality, i.e.,  $p^* \leq d^*$ . In general, this inequality could be strict, and we say that *strong duality* holds if  $p^* = d^*$ . A sufficient condition for having strong duality is the existence of a feasible solution  $X$  for (P) satisfying  $X \succ 0$ . There exist efficient algorithms for solving semidefinite programs (up to any arbitrary precision, and under some technical assumptions). See, e.g., [BTN01, dK02].

**1.4.2. Sums of squares and semidefinite programming.** In this section, we recall an observation already made in [CLR95] showing that the existence of a decomposition of a polynomial as a sum of squares can be modeled with a semidefinite program.



Consider a polynomial  $p \in \mathbb{R}[x]_{2d}$ . Then we have,

$$p \in \Sigma_{2d} \iff p = [x]_d^T M [x]_d \text{ for some } M \succeq 0, \quad (1.16)$$

where  $[x]_d = (x^\alpha)_{|\alpha| \leq d}$  denotes the vector of monomials with degree at most  $d$ .

Indeed, if  $p \in \Sigma_{2d}$  then  $p = \sum_{i=1}^m q_i^2$  for some  $q_i \in \mathbb{R}[x]_d$ . We can write  $q_i = [x]_d^T v_i$  for an appropriate vector  $v_i$ . Then, we obtain  $p = \sum_{i=1}^m q_i^2 = [x]_d^T (\sum_{i=1}^m v_i v_i^T) [x]_d = [x]_d^T M [x]_d$ , where  $M := \sum_{i=1}^m v_i v_i^T$  is a positive semi-definite matrix.

Conversely, assume  $p = [x]_d^T M [x]_d$  with  $M \succeq 0$ . Then  $M = \sum_{i=1}^m v_i v_i^T$  for some vectors  $v_1, \dots, v_m$ . Hence,  $p = \sum_{i=1}^m ([x]_d^T v_i)^2$  is a sum of squares.

So, relation (1.16) shows that testing whether a given polynomial is a sum of squares can be modeled as a semidefinite program.

### 1.5. Approximation hierarchies for polynomial optimization

Based on the result in Putinar's theorem, and motivated by the fact that sums of squares can be modeled via semidefinite programming, Lasserre [Las01b] proposed a hierarchy of approximations  $(f^{(r)})_{r \in \mathbb{N}}$  for problem (1.3). Given an integer  $r \in \mathbb{N}$ , the *quadratic module truncated at degree  $r$*  (generated by the set  $\mathbf{g} = \{g_1, \dots, g_m\}$ ) is defined as

$$\mathcal{M}(\mathbf{g})_r := \left\{ \sum_{i=0}^m \sigma_i g_i : \sigma_i \in \Sigma_{r-\deg(g_i)} \text{ for } i \in \{0, 1, \dots, m\}, \text{ and } g_0 = 1 \right\}. \quad (1.17)$$

The *preordering truncated at degree  $r$*  (generated by the set  $\mathbf{g} = \{g_1, \dots, g_m\}$ ) is defined as

$$\mathcal{T}(\mathbf{g})_r := \left\{ \sum_{J \subseteq [m]} \sigma_J \prod_{i \in J} g_i : \sigma_J \in \Sigma_{r-|J|} \text{ for } J \subseteq \{1, \dots, m\}, \text{ and } g_\emptyset := 1 \right\}.$$

Similarly, the truncated ideal at degree  $r$  generated by the set  $\mathbf{h} = \{h_1, \dots, h_l\}$  is defined as

$$I(\mathbf{h})_r := \left\{ \sum_{i=1}^l p_i h_i : p_i \in \mathbb{R}[x]_{r-\deg(h_i)}, \text{ for } i \in [l] \right\}.$$

Then, one defines the parameter  $f^{(r)}$  as

$$f^{(r)} := \sup \{ \lambda : f - \lambda \in \mathcal{M}(\mathbf{g})_{2r} + I(\mathbf{h})_{2r} \}. \quad (1.18)$$

Clearly,  $f^{(r)} \leq f^{(r+1)} \leq f^*$  for all  $r \in \mathbb{N}$ . The hierarchy of parameters  $f^{(r)}$  is also known as *Lasserre sum-of-squares hierarchy* for problem (1.3).

Under the Archimedean condition, by Putinar's theorem, we have asymptotic convergence of the Lasserre hierarchy:  $f^{(r)} \rightarrow f^*$  as  $r \rightarrow \infty$ . We say that *finite convergence* holds if  $f^{(r)} = f^*$  for some  $r \in \mathbb{N}$ . In general, finite convergence does not hold, as the following example shows.

**Example 1.11.** *Consider the problem*

$$\min x_1 x_2 \quad \text{s.t.} \quad x \in \Delta_3, \text{ i.e., } x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, x_1 + x_2 + x_3 = 1.$$

*The optimal value of this problem is 0 and is attained, for example, in  $x = (0, 0, 1)$ . This problem does not have finite convergence, as we will see in Chapter 2 in the proof of Theorem 2.18.*

**Finite convergence and optimality conditions.** The question of identifying sufficient conditions for which the Lasserre hierarchy of a polynomial optimization problem has finite convergence has been much studied in the literature. For example, in the works by Scheiderer [Sche05, Sche06], Marshall [Mar06, Mar08, Mar09], Kriel and Schweighofer [KS18a, KS18b]. Assume  $f$  is a polynomial nonnegative on a basic closed semialgebraic set  $K$  defined by polynomial inequalities  $\mathbf{g}$ , whose associated quadratic module  $\mathcal{M}(\mathbf{g})$  is Archimedean. Marshall [Mar09, Theorem 1.3] gives a set of algebraic conditions on the zeros of the polynomial  $f$  in the set  $K$ , known as the *Boundary Hessian Condition* (BHC), that guarantees that  $f$  belongs to the quadratic module  $\mathcal{M}(\mathbf{g})$ . Nie [Nie12] shows that (BHC) holds if the natural sufficient optimality conditions hold at all the global minimizers of  $f$  over  $K$  and thus the Lasserre hierarchy has finite convergence in this case. In this section, we recall this result of Nie [Nie12].

We start with a quick recap on these optimality conditions, which we state here for problem (1.3) though they hold in a more general setting (see, e.g., [Bert99]).

Let  $u$  be a local minimizer of problem (1.3) and let

$$J(u) = \{j \in [m] : g_j(u) = 0\}$$

be the index set of the active inequality constraints at  $u$ . We say that the *constraint qualification condition* (CQC) holds at  $u$  if the gradients of the active constraints at  $u$  are linearly independent. Namely,

The vectors in  $\{\nabla g_j(u) : j \in J(u)\} \cup \{\nabla h_i(u) : i \in [l]\}$  are linearly independent. (CQC)

If (CQC) holds at  $u$  then there exist multipliers  $\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_m \in \mathbb{R}$  satisfying

$$\nabla f(u) = \sum_{i=1}^l \lambda_i \nabla h_i(u) + \sum_{j=1}^m \mu_j \nabla g_j(u), \quad (\text{FOOC})$$

$$\mu_1 g_1(u) = 0, \dots, \mu_m g_m(u) = 0, \mu_1 \geq 0, \dots, \mu_m \geq 0. \quad (\text{CC})$$

The condition (FOOC) is known as the *first order optimality condition* and (CC) as the *complementarity condition*. If it holds that

$$\mu_j > 0 \text{ for every } j \in J(u), \quad \mu_j = 0 \text{ for } j \in [m] \setminus J(u), \quad (\text{SCC})$$

then we say that the *strict complementarity condition* (SCC) holds at  $u$ . Define the Lagrangian function

$$L(x) = f(x) - \sum_{i=1}^l \lambda_i h_i(x) - \sum_{j \in J(u)} \mu_j g_j(x).$$

Another necessary condition for  $u$  to be a local minimizer is the *second order necessity condition* (SONC):

$$v^T \nabla^2 L(u) v \geq 0 \text{ for all } v \in G(u)^\perp, \quad (\text{SONC})$$

where  $G(u)$  is the matrix with rows the gradients of the active constraints at  $u$  and  $G(u)^\perp$  is its kernel:

$$G(u)^\perp = \{x \in \mathbb{R}^n : x^T \nabla g_j(u) = 0 \text{ for all } j \in J(u) \text{ and} \\ x^T \nabla h_i(u) = 0 \text{ for all } i \in [l]\}$$

If it holds that

$$v^T \nabla^2 L(u) v > 0 \text{ for all } 0 \neq v \in G(u)^\perp, \quad (\text{SOSC})$$

then we say that the *second order sufficiency condition* (SOSC) holds at  $u$ . The relations between these optimality conditions and the local minimizers are summarized in the following classical result.

**Theorem 1.12** (see, e.g., [Bert99]). *Let  $u$  be a feasible for problem (1.3).*

- (i): *Assume  $u$  is a local minimizer of (1.3) and (CQC) holds at  $u$ . Then the conditions (FOOC), (CC) and (SONC) hold at  $u$ .*
- (ii): *Assume that (FOOC), (SCC) and (SOSC) hold at  $u$ . Then  $u$  is a strict local minimizer of (1.3).*

The relation between the optimality conditions for problem (1.3) and finite convergence of the parameters  $f^{(r)}$  is given by the following result of Nie [Nie12].

**Theorem 1.13** (Nie [Nie12]). *Assume that the Archimedean condition (1.15) holds for the polynomial sets  $\mathbf{g}$  and  $\mathbf{h}$  in problem (1.3). If the constraint qualification condition (CQC), the strict complementarity condition (SCC), and the second order sufficiency condition (SOSC) hold at every global minimizer of (1.3), then the Lasserre hierarchy (1.18) has finite convergence, i.e.,  $f^{(r)} = f^*$  for some  $r \in \mathbb{N}$ .*

We say that a  $x^*$  is a *strict* minimizer of problem (1.3) if it is a global minimizer and it is a strict local minimizer. Note that, under the assumptions of Theorem 1.13, all global minimizers of (1.3) are *strict* minimizers (by Theorem 1.12 (ii)) and thus problem (1.3) has *finitely many* global minimizers. (If not, then there exists a sequence  $(x_i)_i \subseteq K$ , where all  $x_i$  are global minimizers of  $f$  over  $K$ . Under the Archimedean condition,  $K$  is compact and thus this sequence has an accumulation point  $x^* \in K$ . Then  $x^*$  is also a global minimizer, but it is not a strict minimizer, yielding a contradiction.)

### 1.6. Sum-of-squares approximations for $\text{COP}_n$

As mentioned in the Introduction, optimizing over the copositive cone is a hard problem, this motivates to design tractable conic inner approximations for it. One classical cone that is often used as an inner approximation of  $\text{COP}_n$  is the cone  $\text{SPN}_n$ , defined as

$$\text{SPN}_n := \{M \in \mathcal{S}^n : M = P + N \text{ where } P \succeq 0, N \geq 0\}. \quad (1.19)$$

In this section, we explore several hierarchies of conic approximations for  $\text{COP}_n$ , strengthening  $\text{SPN}_n$ , based on sums of squares of polynomials. They are inspired by the positivity certificates (1.8), (1.9), (1.12), and (1.13).

**1.6.1. Cones based on Pólya's nonnegativity certificate.** In view of relation (1.1), a matrix is copositive if the homogeneous polynomial  $x^T M x$  is nonnegative on  $\mathbb{R}_+^n$ . Motivated by the nonnegativity certificate (1.9) in Pólya's theorem, de Klerk and Pasechnik [dKP02] introduced the cones  $\mathcal{C}_n^{(r)}$ , defined as

$$\mathcal{C}_n^{(r)} := \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^r x^T M x \text{ has nonnegative coefficients} \right\} \quad (1.20)$$

for any  $r \in \mathbb{N}$ . Clearly,  $\mathcal{C}_n^{(r)} \subseteq \mathcal{C}_n^{(r+1)} \subseteq \text{COP}_n$ . By Pólya's theorem (Theorem 1.5), the cones  $\mathcal{C}_n^{(r)}$  cover the interior of  $\text{COP}_n$ , i.e.,

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

This follows from the fact that  $M \in \text{int}(\text{COP}_n)$  precisely when  $x^T M x > 0$  for all  $x \in \mathbb{R}_+^n \setminus \{0\}$ . The cones  $\mathcal{C}_n^{(r)}$  were introduced in [dKP02] for approximating the stability number of a graph, as we will see in Chapter 3.

In a similar way, in view of relation (1.2), a matrix is copositive if the homogeneous polynomial  $(x^{\circ 2})^T M x^{\circ 2}$  is globally nonnegative. As mentioned in the introduction, de Klerk and Pasechnik [dKP02] proposed the following cones  $\mathcal{K}_n^{(r)}$  based on the idea of Parrilo [Par00] of certifying matrix copositivity by using certificate (1.8):

$$\mathcal{K}_n^{(r)} := \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^T M x^{\circ 2} \in \Sigma \right\}. \quad (1.21)$$

Clearly,  $\mathcal{C}_n^{(r)} \subseteq \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$ , and thus

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

This inclusion also follows from Reznick's theorem (Theorem 1.2).

The following result by Peña, Vera and Zuluaga [ZVP06] gives information about the structure of the homogeneous polynomials  $f$  for which  $f(x^{\circ 2})$  is

a sum of squares. As a byproduct, this gives the reformulations for the cones  $\mathcal{K}_n^{(r)}$  from relations (1.23) and (1.24) below.

**Theorem 1.14** (Peña, Vera, Zuluaga [ZVP06]). *Let  $f \in \mathbb{R}[x]$  be a homogeneous polynomial with degree  $d$ . Then, the polynomial  $f(x^{\circ 2})$  is a sum of squares if and only if  $f$  admits a decomposition of the form*

$$f = \sum_{\substack{S \subseteq [n], |S| \leq d \\ |S| \equiv d \pmod{2}}} \sigma_S x^S \quad \text{for some } \sigma_S \in \Sigma_{d-|S|}. \quad (1.22)$$

In particular, for any  $r \geq 0$ , we have

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{S \subseteq [n] \\ |S| \leq r+2 \\ |S| \equiv r \pmod{2}}} \sigma_S x^S \quad \text{with } \sigma_S \in \Sigma_{r+2-|S|} \right\}. \quad (1.23)$$

Alternatively, the cones  $\mathcal{K}_n^{(r)}$  may be defined as

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| \leq r+2 \\ |\beta| \equiv r \pmod{2}}} \sigma_\beta x^\beta \quad \text{for some } \sigma_\beta \in \Sigma_{r+2-|\beta|} \right\}, \quad (1.24)$$

where, in (1.23), one replaces square-free monomials by arbitrary monomials. Based on this reformulation of the cones  $\mathcal{K}_n^{(r)}$ , Peña et al. [ZVP06] introduced the cones  $\mathcal{Q}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}$ , defined as

$$\mathcal{Q}_n^{(r)} := \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| = r, r+2}} \sigma_\beta x^\beta \quad \text{for some } \sigma_\beta \in \Sigma_{r+2-|\beta|} \right\}. \quad (1.25)$$

So,  $\mathcal{Q}_n^{(r)}$  is a restrictive version of the formulation (1.24) for the cone  $\mathcal{K}_n^{(r)}$ , in which the decomposition only allows sums of squares of degree 0 and 2. Then, we have

$$\mathcal{C}_n^{(r)} \subseteq \mathcal{Q}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}, \quad (1.26)$$

and thus

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \mathcal{C}_n^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{Q}_n^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}. \quad (1.27)$$

**1.6.2. Lasserre-type approximation cones.** Recall the definitions (1.1) and (1.2) of the copositive cone. Clearly, in (1.1), the nonnegativity condition of the form  $x^T M x$  can be restricted to the simplex  $\Delta_n$  and, in (1.2), the nonnegativity condition of the form  $(x^{\circ 2})^T M x^{\circ 2}$  can be restricted to the unit sphere  $\mathbb{S}^{n-1}$ . Based on these observations, one can now use the positivity certificate (1.12) or (1.13) to certify the nonnegativity on  $\Delta_n$  or  $\mathbb{S}^{n-1}$ . This leads naturally to defining the following cones (as done in [LV22c]): for an integer  $r \geq 2$ ,

$$\text{LAS}_{\Delta_n}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x \in \mathcal{M}(\mathbf{x})_r + I_{\Delta_n} \right\}, \quad (1.28)$$

$$\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x \in \mathcal{T}(\mathbf{x})_r + I_{\Delta_n} \right\}, \quad (1.29)$$

and for an integer  $r \geq 4$ ,

$$\text{LAS}_{\mathbb{S}^{n-1}}^{(r)} = \left\{ M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \in \Sigma_r + I_{\mathbb{S}^{n-1}} \right\}. \quad (1.30)$$

Clearly, we have

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)},$$

and, by Putinar's theorem (Theorem 1.9),

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}, \quad \text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \text{LAS}_{\mathbb{S}^{n-1}}^{(r)}. \quad (1.31)$$

Here, we are using the well-known fact that the quadratic modules  $\mathcal{M}(\mathbf{x}) + I_{\Delta_n}$  and  $\Sigma + I_{\mathbb{S}^{n-1}}$  are Archimedean. We refer to relation (2.17) for an argument that  $\mathcal{M}(\mathbf{x}) + I_{\Delta_n}$  is Archimedean. The quadratic module  $\Sigma + I_{\mathbb{S}^{n-1}}$  is Archimedean because  $\sum_{i=1}^n x_i^2 - 1 \in I_{\mathbb{S}^{n-1}}$ .

In the next chapter, we will study the exact relation between these approximation cones. In particular, we will show that the conic hierarchies  $\mathcal{K}_n^{(r)}$ ,  $\text{LAS}_{\mathcal{T}, \Delta_n}^{(r)}$  and  $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$  are equivalent (see relation (2.1) and Theorem 2.10).

## Exactness of sum-of-squares approximations for $\text{COP}_n$

*The main results of this chapter are from my joint work [LV22c] with Monique Laurent. However, the language used here is slightly different. Selected results from my works [LV22a] and [LV22b] with Monique Laurent are also included as will be specified throughout. In particular, the results from Section 2.1 are from [LV22b].*

In this chapter, we study the question of whether the hierarchies of cones introduced in Section 1.6 cover the full copositive cone  $\text{COP}_n$ . For this, we first study the relation between these cones and show the following links: for any integer  $r \geq 2$ , we have

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r-2)} = \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)} = \text{LAS}_{\mathbb{S}^{n-1}}^{(2r)}. \quad (2.1)$$

(see Theorem 2.10). We are particularly interested in analyzing the conic approximations  $\mathcal{K}_n^{(r)}$ , which are equivalent to the conic approximations  $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$  and  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ , in view of relation (2.1).

The cone  $\mathcal{K}_n^{(0)}$  is known to be equal to the cone  $\text{SPN}_n$  from (1.19) (see [Par00]):

$$\mathcal{K}_n^{(0)} = \text{SPN}_n. \quad (2.2)$$

Diananda [Dian62] showed that the equality  $\text{SPN}_n = \text{COP}_n$  holds for  $n \leq 4$ . Then,

$$\text{COP}_n = \mathcal{K}_n^{(0)} \text{ for } n \leq 4. \quad (2.3)$$

It is known that the inclusion  $\mathcal{K}_5^{(0)} \subseteq \text{COP}_5$  is strict. For instance, the following matrix, known as the *Horn matrix*,

$$H = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{pmatrix} \quad (2.4)$$

is copositive, but it does not belong to the cone  $\mathcal{K}_5^{(0)}$  (a proof of this well-known fact will be shown in Example 5.28) in Chapter 5. On the other hand,

Parrilo [Par00] showed that  $H$  belongs to the cone  $\mathcal{K}_5^{(1)}$ .

The notion of positive diagonal scaling plays a crucial role in the analysis of the exactness of the conic approximations  $\mathcal{K}_n^{(r)}$ . Let us first introduce the set of positive diagonal matrices  $\mathcal{D}_{++}^n$ .

$$\mathcal{D}_{++}^n := \{D \in \mathcal{S}^n : D \text{ is a diagonal matrix with } D_{ii} > 0 \text{ for all } i \in [n]\}.$$

Given a symmetric matrix  $M \in \mathcal{S}^n$  a positive diagonal scaling of  $M$  is a matrix of the form  $DMD$ , where  $D \in \mathcal{D}_{++}^n$ . Clearly, any positive diagonal scaling of a copositive matrix remains a copositive matrix. However, this operation does *not* preserve the cone  $\mathcal{K}_n^{(r)}$  for  $r \geq 1$  (see [DDGH13]). For instance,  $H \in \mathcal{K}_5^{(1)}$ , but not every positive diagonal scaling of  $H$  belongs to  $\mathcal{K}_5^{(1)}$  (see Theorem 5.6 for a characterization of the diagonal matrices  $D$  for which  $DHD \in \mathcal{K}_5^{(1)}$ ). Moreover, it is shown in [DDGH13] that the set of diagonal scalings of the Horn matrix is not contained in a single cone  $\mathcal{K}_5^{(r)}$ . As a consequence, the inclusion  $\mathcal{K}_n^{(r)} \subseteq \text{COP}_n$  is strict for every  $n \geq 5$ ,  $r \geq 0$ . Hence, the remaining question is whether the union of the cones  $\mathcal{K}_n^{(r)}$  covers the full copositive cone  $\text{COP}_n$ .

**Question 2.1.** *Does the equality  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} = \text{COP}_n$  hold for some  $n \geq 5$ ?*

In this chapter, we show that for  $n \geq 6$  the inclusion  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$  is strict (see Theorem 2.7). The remaining case  $n = 5$  is answered affirmatively in this thesis.

**Theorem 2.2.** *We have  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)} = \text{COP}_5$ .*

The proof of this result is divided into two main steps. The first step is to reduce the problem to the positive diagonal scalings of the Horn matrix. This is the main result of this chapter.

**Theorem 2.3.** *Equality  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)} = \text{COP}_5$  holds if and only if  $DHD$  belongs to  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$  for all positive diagonal matrices  $D$ .*

The second step, i.e., that every positive diagonal scaling of the Horn matrix belongs to  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ , is shown in Chapter 6.

We now summarize the main ingredients of the proof of Theorem 2.3. In order to show that any  $5 \times 5$  copositive matrix lies in some  $\mathcal{K}_5^{(r)}$ , we can restrict our attention to copositive matrices that lie on the boundary  $\partial \text{COP}_5$  of the copositive cone, since, as saw earlier,  $\text{int}(\text{COP}_5) \subseteq \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ . Moreover, it suffices to consider matrices that lie on an extreme ray of  $\text{COP}_5$ .

A crucial ingredient for the proof of Theorem 2.3 is the fact that all the extreme rays of the cone  $\text{COP}_5$  are known. They have been characterized by Hildebrand [Hil12], who defined the following matrices



$$T(\psi) = \begin{pmatrix} 1 & -\cos \psi_4 & \cos(\psi_4 + \psi_5) & \cos(\psi_2 + \psi_3) & -\cos \psi_3 \\ -\cos \psi_4 & 1 & -\cos \psi_5 & \cos(\psi_5 + \psi_1) & \cos(\psi_3 + \psi_4) \\ \cos(\psi_4 + \psi_5) & -\cos \psi_5 & 1 & -\cos \psi_1 & \cos(\psi_1 + \psi_2) \\ \cos(\psi_2 + \psi_3) & \cos(\psi_5 + \psi_1) & -\cos \psi_1 & 1 & -\cos \psi_2 \\ -\cos \psi_3 & \cos(\psi_3 + \psi_4) & \cos(\psi_1 + \psi_2) & -\cos \psi_2 & 1 \end{pmatrix}, \quad (2.5)$$

where  $\psi \in \mathbb{R}^5$ , and proved the following theorem.

**Theorem 2.4** ([Hil12]). *Let  $M \in \text{COP}_5$  be an extreme matrix, and assume that  $M$  is neither an element of  $\mathcal{K}_5^{(0)}$  nor a positive diagonal scaling (of a row/column permutation) of the Horn matrix. Then  $M$  is of the form*

$$M = P \cdot D \cdot T(\psi) \cdot D \cdot P^T,$$

where  $P$  is a permutation matrix,  $D \in \mathcal{D}_{++}^5$ , and the quintuple  $\psi$  is an element of the set

$$\Psi = \left\{ \psi \in \mathbb{R}^5 : \sum_{i=1}^5 \psi_i < \pi, \psi_i > 0 \text{ for } i \in [5] \right\}. \quad (2.6)$$

In summary, the extreme matrices  $M$  of  $\text{COP}_5$  can be divided into three categories:

- (i):  $M \in \mathcal{K}_n^{(0)}$ ,
- (ii):  $M$  is (up to row/column permutation) a positive diagonal scaling of the Horn matrix,
- (iii):  $M$  is (up to row/column permutation) a positive diagonal scaling of a matrix  $T(\psi)$  for some  $\psi \in \Psi$ .

Our main result in this chapter is to show that every matrix from the third category of extreme matrices of  $\text{COP}_5$  belongs to some cone  $\text{LAS}_{\Delta_5}^{(r)}$  and thus, in view of (2.1), to some cone  $\mathcal{K}_5^{(r)}$ .

**Theorem 2.5.** *Let  $D \in \mathcal{D}_{++}$  be a positive diagonal matrix. Then, for all  $\psi \in \Psi$ , we have  $D \cdot T(\psi) \cdot D \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_5}^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ .*

In view of Theorem 2.4, Theorem 2.3 directly follows from Theorem 2.5. The proof of Theorem 2.5 forms the main technical part of the chapter, which, as we will explain below, relies on following an optimization approach.

**Organization of the chapter.** In Section 2.1, we construct copositive matrices that do not lie in any cone  $\mathcal{K}_n^{(r)}$  for  $n \geq 6$ . For  $n \geq 7$ , these matrices can be taken with an all-ones diagonal, thus disproving a conjecture from [DDGH13]. In Section 2.2, we will investigate the relation between the cones  $\text{LAS}_{\Delta_n}^{(r)}$ ,  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ ,  $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$ ,  $\mathcal{K}_n^{(r)}$  and  $\mathcal{Q}_n^{(r)}$  defined in Section 1.6 for approximating  $\text{COP}_n$ . In particular, we will show relation (2.1). In Section 2.3, we analyze the membership in the cones  $\text{LAS}_{\Delta_n}^{(r)}$ , and we characterize the cases for which the inclusion  $\text{LAS}_{\Delta_n}^{(r)} \subseteq \text{COP}_n$  is strict. In Section 2.4, we show Theorem 2.5. For this, we use optimization techniques for giving sufficient

conditions on a copositive matrix  $M$  such that  $M$  and all its diagonal scalings belong to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ .

### 2.1. Constructing copositive matrices outside $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$

In this section, we show a result that permits to construct copositive matrices that do not belong to any of the cones  $\mathcal{K}_n^{(r)}$ . In particular, we show that the inclusion  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$  is strict for  $n \geq 6$ . We also disprove a conjecture from [DDGH13] claiming that every copositive matrix with an all-ones diagonal belongs to some cone  $\mathcal{K}_n^{(r)}$ .

We start with a preliminary result on sums of squares of polynomials.

**Lemma 2.6.** *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 polynomials  $q_i \in \mathbb{R}[x]$  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  $L = \min\{L_i : i \in [m]\}$ . Note that there is no monomial with degree less than  $2L$  in  $\sum_i q_i^2 = f$  and  $f_{2L} = \sum_{i=1}^m (a_i^{(L)})^2 \neq 0$ . Hence, it follows that  $f_r = f_{2L}$  is a sum of squares.  $\square$

**Theorem 2.7.** *Let  $M_1 \in \text{COP}_n$  and  $M_2 \in \text{COP}_m$  be two copositive matrices. Assume that  $M_1 \notin \mathcal{K}_n^{(0)}$  and that there exists  $0 \neq z \in \mathbb{R}_+^m$  such that  $z^T M_2 z = 0$ . Then we have*

$$\left( \begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array} \right) \in \text{COP}_{n+m} \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_{n+m}^{(r)}. \quad (2.7)$$

PROOF. Assume by contradiction  $M_1 \oplus M_2 \in \mathcal{K}_{n+m}^{(r)}$ , i.e., the polynomial  $(P_{M_1}(x) + P_{M_2}(y))(\sum_{i=1}^n x_i^2 + \sum_{j=1}^m y_j^2)^r$  is a sum of squares. Here, for convenience, we denote the  $n+m$  variables as  $x_i$  ( $i \in [n]$ ) and  $y_j$  ( $j \in [m]$ ) and we set  $P_{M_1}(x) = (x^{\circ 2})^T M_1 x^{\circ 2}$  and  $P_{M_2}(y) = (y^{\circ 2})^T M_2 y^{\circ 2}$ . Write  $z = y^{\circ 2}$  for some  $y \in \mathbb{R}^m$ , so that  $P_{M_2}(y) = 0$ , and  $c := \sum_{j=1}^m y_j^2 > 0$ . Then, the polynomial  $f(x) := P_{M_1}(x)(\sum_{i=1}^n x_i^2 + c)^r$  is a sum of squares. By decomposing  $f$  as a sum of homogeneous polynomials, we see that its least degree homogeneous part is the polynomial  $c^r P_{M_1}(x)$ , with degree  $4$ . Using Lemma 2.6, we obtain that  $c^r P_{M_1}(x)$  is a sum of squares, i.e,  $M_1 \in \mathcal{K}_n^{(0)}$ , yielding a contradiction.  $\square$

Now we give explicit examples of copositive matrices of size  $n \geq 6$  that do not belong to any of the cones  $\mathcal{K}_n^{(r)}$ .

**Example 2.8.** Let  $M_1 = H$  be the Horn matrix, known to be copositive with  $H \notin \mathcal{K}_n^{(0)}$ . For the matrix  $M_2$  we first consider the  $1 \times 1$  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 Proposition 2.7 (taking  $z = 1$  and  $z = (1, 1)$ , respectively), we obtain

$$\left( \begin{array}{c|c} H & 0 \\ \hline 0 & 0 \end{array} \right) \in \text{COP}_6 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_6^{(r)}, \quad \left( \begin{array}{c|cc} H & & 0 \\ \hline & 1 & -1 \\ & -1 & 1 \end{array} \right) \in \text{COP}_7 \setminus \bigcup_{r \in \mathbb{N}} \mathcal{K}_7^{(r)}. \quad (2.8)$$

The leftmost matrix in (2.8) is copositive, it has all its diagonal entries equal to 0 or 1, and it does not belong to any of the cones  $\mathcal{K}_6^{(r)}$ . Selecting for  $M_2$  the zero matrix of size  $m \geq 1$  gives a matrix in  $\text{COP}_n \setminus \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$  for any size  $n \geq 6$ . The rightmost matrix in (2.8) is copositive, it has all its diagonal entries equal to 1, and it 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 an all-ones diagonal for any size  $n \geq 7$ . In contrast, it was shown in [DDGH13] that any copositive  $5 \times 5$  matrix with an all-ones diagonal belongs to  $\mathcal{K}_5^{(1)}$ . The situation for the case of  $6 \times 6$  copositive matrices remains open.

**Question 2.9.** Is it true that any  $6 \times 6$  copositive matrix with an all-ones diagonal belongs to  $\mathcal{K}_6^{(r)}$  for some  $r \in \mathbb{N}$ ?

## 2.2. Links between the approximation cones for COP<sub>n</sub>

In this section, we show the relationships from (2.1) between the cones  $\mathcal{K}_n^{(r)}$ ,  $\text{LAS}_{\Delta_n}^{(r)}$ ,  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  and  $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$  introduced in Section 1.6. In addition, we highlight the relationship to the cones  $\mathcal{Q}_n^{(r)}$  introduced in [PVZ07] and point out how these cones can all be seen as distinct variations within a common framework.

**Theorem 2.10.** Let  $r \geq 2$  and  $n \geq 1$ , then we have

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r-2)} = \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)} = \text{LAS}_{\mathbb{S}^{n-1}}^{(2r)}.$$

We begin with observing that in the definition (1.29) of the cone  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  we may assume that the summation only involves sets  $S \subseteq [n]$  with  $|S| \equiv r \pmod{2}$ .

**Lemma 2.11.** We have

$$\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{S \subseteq [n], |S| \leq r \\ |S| \equiv r \pmod{2}}} \sigma_S x^S + q \text{ with } \sigma_S \in \Sigma_{r-|S|}, q \in I_{\Delta_n} \right\}.$$

PROOF. To see this, consider a term  $x^S \sigma_S$ , where  $|S| \leq r$ ,  $|S| \not\equiv r \pmod{2}$  and  $\sigma_S \in \Sigma_{r-|S|}$ . Then  $|S| \leq r-1$ ,  $\deg(\sigma_S) \leq r-|S|-1$  and thus, modulo the ideal  $I_{\Delta_n}$ , we can replace  $x^S \sigma_S$  by  $x^S \sigma_S (\sum_{i=1}^n x_i)$ . Now expand this expression as  $\sum_{i \in S} x^{S \setminus \{i\}} \cdot \sigma_S x_i^2 + \sum_{i \in [n] \setminus S} x^{S \cup \{i\}} \sigma_S$ . So each term in this summation is of the form  $x^T \sigma_T$  with  $|T| \leq r$ ,  $|T| \equiv r \pmod{2}$ , and  $\deg(\sigma_T) \leq r - |T|$ .  $\square$

Note the similarity between the description of  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  in Lemma 2.11 and that of  $\mathcal{K}_n^{(r-2)}$  in relation (1.23). The difference lies in the fact that for  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  we have a representation of  $x^T M x$  modulo the ideal  $I_{\Delta_n}$ , while for  $\mathcal{K}_n^{(r-2)}$  we have a representation of  $(\sum_{i=1}^n x_i)^{r-2} x^T M x$ . The next lemma (whose main idea was already used, e.g., in [dKLP05]) gives a simple trick, useful to navigate between these two types of representations.

**Lemma 2.12.** *Let  $f, g \in \mathbb{R}[x]$  and assume  $f$  is homogeneous. The following assertions hold.*

- (i): *If  $(\sum_{i=1}^n x_i)^r f(x) = g(x)$ , then  $f - g \in I_{\Delta_n}$ .*
- (ii): *Let  $\deg(f) = d$ ,  $\deg(g) = d + r$  ( $r \in \mathbb{N}$ ), and define*

$$\tilde{g}(x) = \left( \sum_{i=1}^n x_i \right)^{d+r} g\left(x / \left( \sum_{i=1}^n x_i \right)\right).$$

*Then,  $\tilde{g}$  is a homogeneous polynomial of degree  $d + r$ . Moreover, if  $f - g \in I_{\Delta_n}$ , then  $(\sum_{i=1}^n x_i)^r f(x) = \tilde{g}(x)$ .*

PROOF. The assertion (i) follows by expanding  $(\sum_{i=1}^n x_i)^r$  as the sum

$$\left( \sum_{i=1}^n x_i \right)^r = \left( \sum_{i=1}^n x_i - 1 + 1 \right)^r = 1 + \left( \sum_{i=1}^n x_i - 1 \right) \left( \sum_{k=1}^r \binom{r}{k} \left( \sum_{i=1}^n x_i - 1 \right)^{k-1} \right).$$

We now show (ii). The claim that  $\tilde{g}$  is a homogeneous polynomial of degree  $d+r$  is easy to check. Assume now  $f - g \in I_{\Delta_n}$ . By evaluating  $f - g$  at  $x / (\sum_{i=1}^n x_i)$ , we obtain  $f(x / (\sum_{i=1}^n x_i)) = g(x / (\sum_{i=1}^n x_i))$ . As  $f$  is homogeneous of degree  $d$  this implies  $f(x) = (\sum_{i=1}^n x_i)^d g(x / (\sum_{i=1}^n x_i))$ , and the result follows after multiplying both sides by  $(\sum_{i=1}^n x_i)^r$ .  $\square$

We will also use the following simple fact.

**Lemma 2.13.** *Let  $\sigma \in \Sigma_k$  and define  $\tilde{\sigma}(x) = (\sum_{i=1}^n x_i)^k \sigma(x / (\sum_{i=1}^n x_i))$ . Then  $\tilde{\sigma}$  is a homogeneous polynomial of degree  $k$ . Moreover,*

- (i) *If  $k \equiv \deg(\sigma) \pmod{2}$ , then  $\tilde{\sigma} \in \Sigma$ .*
- (ii) *If  $k \not\equiv \deg(\sigma) \pmod{2}$ , then  $\tilde{\sigma} = (\sum_{i=1}^n x_i) \hat{\sigma}$ , where  $\hat{\sigma} \in \Sigma$ .*

PROOF. Note that  $\tilde{\sigma} = (\sum_{i=1}^n x_i)^{k-\deg(\sigma)} \sigma'$ , where

$$\sigma' := \left( \sum_{i=1}^n x_i \right)^{\deg(\sigma)} \sigma \left( x / \left( \sum_{i=1}^n x_i \right) \right)$$

is a homogeneous polynomial with degree  $\deg(\sigma)$ . It suffices now to observe that  $(\sum_{i=1}^n x_i)^{k-\deg(\sigma)}$  is a square if  $k - \deg(\sigma)$  is even, and it is a square times  $(\sum_i x_i)$  if  $k - \deg(\sigma)$  is odd.  $\square$

Using these two lemmas, we can now relate the two cones  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  and  $\mathcal{K}_n^{(r-2)}$ .

**Lemma 2.14.** *For any  $r \geq 2$ , we have  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)} = \mathcal{K}_n^{(r-2)}$ .*

PROOF. First assume  $M \in \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ . Using Lemma 2.11, we have a decomposition of the form  $x^T M x = g(x) + q(x)$ , where  $q \in I_{\Delta_n}$  and  $g(x) = \sum_{|S| \leq r, |S| \equiv r \pmod{2}} \sigma_S x^S$ , with  $\sigma_S \in \Sigma_{r-|S|}$ . Using Lemma 2.12(ii), we get

$$\left( \sum_{i=1}^n x_i \right)^{r-2} x^T M x = \left( \sum_{i=1}^n x_i \right)^r g\left( \frac{x}{\sum_i x_i} \right) = \sum_{\substack{|S| \leq r \\ |S| \equiv r}} x^S \underbrace{\left( \sum_{i=1}^n x_i \right)^{r-|S|} \sigma_S \left( \frac{x}{\sum_i x_i} \right)}_{=\tilde{\sigma}_S(x)}.$$

As  $r - |S| \equiv \deg(\sigma_S) \pmod{2}$ , we have  $\tilde{\sigma}_S \in \Sigma_{r-|S|}$  by Lemma 2.13(i). In view of relation (1.23), this shows that  $M \in \mathcal{K}_n^{(r-2)}$ .

Conversely, assume  $M \in \mathcal{K}_n^{(r-2)}$ . Then, in view of (1.23), we have a decomposition of the form

$$\left( \sum_{i=1}^n x_i \right)^{r-2} x^T M x = \sum_{\substack{|S| \leq r \\ |S| \equiv r \pmod{2}}} \sigma_S x^S,$$

where  $\sigma_S \in \Sigma_{r-|S|}$ . By applying Lemma 2.12(i), we obtain

$$x^T M x = \sum_{\substack{|S| \leq r \\ |S| \equiv r \pmod{2}}} \sigma_S x^S + q,$$

where  $q \in I_{\Delta_n}$ . Combining with Lemma 2.11, this shows  $M \in \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ .  $\square$

To complete the proof of Theorem 2.10 we now establish the relation to the cone  $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$ , which follows from the following result in [dKLP05].

**Proposition 2.15** ([dKLP05]). *Let  $f$  be a homogeneous polynomial of degree  $2d$  and  $r \in \mathbb{N}$ . Then,  $f\left(\sum_{i=1}^n x_i^2\right)^r \in \Sigma$  if and only if*

$$f = \sigma + u\left(1 - \sum_{i=1}^n x_i^2\right), \quad \text{for some } \sigma \in \Sigma_{2r+2d} \text{ and } u \in \mathbb{R}[x].$$

In particular, for any  $r \geq 2$ , we have

$$\text{LAS}_{\mathbb{S}^{n-1}}^{(2r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i^2 \right)^{r-2} (x^{\circ 2})^T M x^{\circ 2} \in \Sigma \right\} = \mathcal{K}_n^{(r-2)}. \quad (2.9)$$

We conclude this section with a reformulation for the cone  $\text{LAS}_{\Delta_n}^{(r)}$  in the same vein as the reformulation of  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$  in Lemma 2.11.

**Lemma 2.16.** *Let  $r \geq 2$ . If  $r$  is odd, then we have*

$$\text{LAS}_{\Delta_n}^{(r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^{r-2} x^T M x = \sum_{i=1}^n \sigma_i x_i \text{ with } \sigma_i \in \Sigma_{r-1} \right\}. \quad (2.10)$$

If  $r$  is even and  $r \geq 4$ , then we have  $\text{LAS}_{\Delta_n}^{(r)} = \text{LAS}_{\Delta_n}^{(r-1)}$ .

PROOF. The proof is similar to that of Lemma 2.11, except we now have a summation that involves only sets  $S \subseteq [n]$  with  $|S| \leq 1$ . We spell out the details for clarity. Consider first the case when  $r$  is odd. Assume that  $M \in \text{LAS}_{\Delta_n}^{(r)}$ , so that  $x^T M x = \sigma_0 + \sum_{i=1}^n \sigma_i x_i + q$ , where  $q \in I_{\Delta}$ ,  $\sigma_0 \in \Sigma_r$ , and  $\sigma_i \in \Sigma_{r-1}$ . Combining Lemma 2.12(ii) and Lemma 2.13 we obtain a decomposition as in (2.10). Conversely, starting from a decomposition as in (2.10) we get a decomposition as in (1.28) by applying Lemma 2.12(i).

Consider now the case  $r \geq 4$  even. Assume  $M \in \text{LAS}_{\Delta_n}^{(r)}$ , we show that  $M \in \text{LAS}_{\Delta_n}^{(r-1)}$ . Starting from a decomposition as in (1.28) and using as above Lemma 2.12(i) and Lemma 2.13, we obtain a decomposition

$$\left( \sum_{j=1}^n x_j \right)^{r-2} x^T M x = \tilde{\sigma}_0 + \left( \sum_{j=1}^n x_j \right) \sum_{i=1}^n \tilde{\sigma}_i x_i,$$

where  $\tilde{\sigma}_0 \in \Sigma_r$  and  $\tilde{\sigma}_i \in \Delta_{r-1}$ . From this, it follows that the polynomial  $\sum_{j=1}^n x_j$  divides  $\tilde{\sigma}_0$ , which implies its square divides  $\tilde{\sigma}_0$ . Then we can divide out by  $\sum_{j=1}^n x_j$  and obtain an expression as in (2.10) (replacing  $r$  by  $r-1$ ), that certifies membership of  $M$  in  $\text{LAS}_{\Delta_n}^{(r-1)}$ .  $\square$

We finish by observing that the cones  $\mathcal{C}_n^{(r)}$  and  $\mathcal{Q}_n^{(r)}$ , introduced in (1.20) and (1.25) and defined by requiring a special decomposition of the polynomial  $(\sum_{i=1}^n x_i)^r x^T M x$ , can be equivalently defined, in view of Lemmas 2.12 and 2.13, by requiring an analogous decomposition of the polynomial  $x^T M x$  modulo the ideal  $I_{\Delta_n}$ .

**Lemma 2.17.** *For  $n \geq 1$ ,  $r \geq 0$  we have*

$$\mathcal{C}_n^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta|=r+2}} c_\beta x^\beta + q \text{ for } c_\beta \geq 0 \text{ and } q \in I_{\Delta_n} \right\}, \quad (2.11)$$

$$\mathcal{Q}_n^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta|=r, r+2}} \sigma_\beta x^\beta + q \text{ for } \sigma_\beta \in \Sigma_{r+2-|\beta|} \text{ and } q \in I_{\Delta_n} \right\}. \quad (2.12)$$

To conclude, we illustrate how membership in the cones  $\text{LAS}_{\Delta_n}^{(r)}$ ,  $\text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ ,  $\mathcal{C}_n^{(r)}$ , and  $\mathcal{Q}_n^{(r)}$  can also be viewed as ‘restrictive’ versions of membership in the cone  $\mathcal{K}_n^{(r-2)}$ . Indeed, as we saw above,  $\mathcal{K}_n^{(r-2)} = \text{LAS}_{\Delta_n, \mathcal{T}}^{(r)}$ , and thus a matrix  $M$  belongs to  $\mathcal{K}_n^{(r-2)}$  if and only if the form  $x^T M x$  has a decomposition of the form (2.13).

On the other hand, membership in the cones  $\text{LAS}_{\Delta_n}^{(r)}$ ,  $\mathcal{C}_n^{(r-2)}$ , and  $\mathcal{Q}_n^{(r-2)}$  corresponds to restricting to decompositions that allow only some of the terms appearing in (2.13):

$$\underbrace{\sigma_0 + \sum_{i=1}^n x_i \sigma_i + \cdots + \sum_{\beta \in \mathbb{N}^n, |\beta|=r-2} x^\beta \sigma_\beta}_{\text{for cones } \text{LAS}_{\Delta_n}^{(r)}} + \overbrace{\sum_{\beta \in \mathbb{N}^n, |\beta|=r-2} x^\beta \sigma_\beta + \sum_{\beta \in \mathbb{N}^n, |\beta|=r} x^\beta c_\beta}^{\text{for cones } \mathcal{Q}_n^{(r-2)}} + \underbrace{q \left( \sum_{i=1}^n x_i - 1 \right)}_{\text{for cones } \begin{cases} \text{LAS}_{\Delta_n}^{(r)} \\ \mathcal{Q}_n^{(r-2)} \\ \mathcal{C}_n^{(r-2)} \end{cases}}. \quad (2.13)$$

### 2.3. Characterizing the equality $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} = \text{COP}_n$

In this section, we characterize the matrix sizes  $n$  for which the hierarchy of cones  $\text{LAS}_{\Delta_n}^{(r)}$  covers the full copositive cone  $\text{COP}_n$ .

**Theorem 2.18.** *We have  $\text{COP}_2 = \text{LAS}_{\Delta_2}^{(3)}$  and for  $n \geq 3$ , the inclusion  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} \subseteq \text{COP}_n$  is strict.*

PROOF. First, assume  $M = \begin{pmatrix} a & c \\ c & b \end{pmatrix} \in \text{COP}_2$ , we show  $M \in \text{LAS}_{\Delta_2}^{(3)}$ . Note that  $a, b \geq 0$  and  $c \geq -\sqrt{ab}$  (using the fact that  $u^T M u \geq 0$  with  $u = (1, 0)$ ,  $(0, 1)$ , and  $(\sqrt{b}, \sqrt{a})$ ). Then, we can write

$$x^T M x = (\sqrt{a}x_1 - \sqrt{b}x_2)^2 + 2(c + \sqrt{ab})x_1x_2,$$

which, modulo the ideal  $I_{\Delta_2}$ , is equal to

$$(\sqrt{a}x_1 - \sqrt{b}x_2)^2(x_1 + x_2) + 2(c + \sqrt{ab})(x_2^2x_1 + x_1^2x_2),$$

thus showing  $M \in \text{LAS}_{\Delta_2}^{(3)}$ .

For  $n = 3$ , the matrix

$$M := \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (2.14)$$

is copositive (since nonnegative), but does not belong to any of the cones  $\text{LAS}_{\Delta_3}^{(r)}$ . To see this, assume, by way of contradiction, that  $M \in \text{LAS}_{\Delta_3}^{(r)}$  for some  $r \in \mathbb{N}$ . Then, the polynomial  $x^T M x = 2x_1x_2$  can be written as

$$2x_1x_2 = \sigma_0 + \sum_{i=1}^3 x_i \sigma_i + q \left( \sum_{i=1}^3 x_i - 1 \right), \quad (2.15)$$

for some  $\sigma_i \in \Sigma$  for  $i = 0, 1, 2, 3$  and  $q \in \mathbb{R}[x]$ . For a scalar  $t \in (0, 1)$ , define the vector  $u_t := (t, 0, 1 - t) \in \Delta_3$ . Now we evaluate equation (2.15) at  $x + u_t$  and obtain

$$\begin{aligned} 2x_1x_2 + 2tx_2 &= \sigma_0(x + u_t) + (x_1 + t)\sigma_1(x + u_t) + x_2\sigma_2(x + u_t) \\ &\quad + (x_3 + 1 - t)\sigma_3(x + u_t) + q(x + u_t)(x_1 + x_2 + x_3) \end{aligned}$$

for any fixed  $t \in (0, 1)$ . We compare the coefficients of the polynomials in  $x$  at both sides of the above identity. Observe that there is no constant term on the left hand side, so  $\sigma_0(u_t) + t\sigma_1(u_t) + (1 - t)\sigma_3(u_t) = 0$ , which implies  $\sigma_i(u_t) = 0$  for  $i = 0, 1, 3$  as  $\sigma_i \in \Sigma$  and thus  $\sigma_i(u_t) \geq 0$ . Then, for  $i = 0, 1, 3$ , the polynomial  $\sigma_i(x + u_t)$  has no constant term, and thus it has no linear terms. Now, by comparing the coefficient of  $x_1$  at both sides, we get  $q(u_t) = 0$ . Finally, by comparing the coefficient of  $x_2$  at both sides, we get  $t = \sigma_2(u_t)$  for all  $t \in (0, 1)$ . This implies  $\sigma_2(u_t) = t$  as polynomial in the variable  $t$ . This is a contradiction because  $\sigma_2(u_t)$  is a sum of squares in  $t$ .  $\square$

By Theorems 2.10 and 2.18, we have  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ , with equality if  $n = 2$ . This inclusion is strict for any  $n \geq 3$ . Indeed, the matrix  $M$  in (2.14) is an example of a matrix that does not belong to any cone  $\text{LAS}_{\Delta_3}^{(r)}$  while it belongs to the cone  $\mathcal{K}_3^{(0)}$  (because  $M$  is copositive and  $\text{COP}_3 = \mathcal{K}_3^{(0)}$ ).

Following a similar argument as the one used for showing that the matrix in (2.14) does not belong to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_3}^{(r)}$ , we can show that the Horn matrix does not belong to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_5}^{(r)}$ . The full proof can be found in ([LV22c], Lemma 3.10).

**Proposition 2.19.** *We have  $H \notin \text{LAS}_{\Delta_5}^{(r)}$  for any  $r \in \mathbb{N}$ .*



We just saw two examples of copositive matrices that do not belong to any cone  $\text{LAS}_{\Delta_n}^{(r)}$ . In both cases, the structure of the *infinitely many* zeros plays a crucial role. We will now discuss some tools that can be used to show membership in some cone  $\text{LAS}_{\Delta_n}^{(r)}$  in the case when the quadratic form  $x^T M x$  has *finitely many* zeros in  $\Delta_n$ . These tools will be useful for showing that the matrices  $T(\psi)$  from (2.5) belong to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_5}^{(r)}$ , and thus to  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ .

## 2.4. Main result

Recall that, if a matrix  $M$  lies in the interior of the cone  $\text{COP}_n$ , then it belongs to some cone  $\text{LAS}_{\Delta_n}^{(r)}$  (see relation (1.31)). Therefore, we now assume that  $M$  lies on the boundary of  $\text{COP}_n$ , denoted by  $\partial\text{COP}_n$ .

Consider a matrix  $M \in \partial\text{COP}_n$ . The objective of this section is to give sufficient conditions on  $M$  that permit us to conclude that every positive diagonal scaling of  $M$  belongs to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ . This will be very useful since we will show that the matrices  $T(\psi)$  ( $\psi \in \Psi$ ) satisfy these sufficient conditions and thus we will be able to conclude the proof of Theorem 2.5. Our strategy is to apply the result from Nie's theorem (Theorem 1.13) to the setting of standard quadratic programs. Let us define the following standard quadratic program:

$$\min\{x^T M x : x \in \Delta_n\} \quad (\text{SQP}_M)$$

and the corresponding Lasserre hierarchy

$$p_M^{(r)} = \sup \left\{ \lambda : x^T M x - \lambda \in \mathcal{M}(\mathbf{x})_{2r} + I_{\Delta_n} \right\}. \quad (2.16)$$

Note the optimal value of  $(\text{SQP}_M)$  is zero as  $M \in \partial\text{COP}_n$ . Now, we will apply Nie's theorem (Theorem 1.13) to problem  $(\text{SQP}_M)$ . The set  $K = \Delta_n$  indeed satisfies the Archimedean condition. For this, note that, for any  $i \in [n]$ , we have

$$\begin{aligned} 1 - x_i &= 1 - \sum_{k=1}^n x_k + \sum_{k \in [n] \setminus \{i\}} x_k, \\ 1 - x_i^2 &= \frac{(1 + x_i)^2}{2} (1 - x_i) + \frac{(1 - x_i)^2}{2} (1 + x_i). \end{aligned} \quad (2.17)$$

This implies  $n - \sum_{i=1}^n x_i^2 \in \mathcal{M}(\mathbf{x}) + I_{\Delta_n}$ , thus showing that the Archimedean condition holds. By [Mar03, Theorem 3.1], the feasible region of the Lasserre hierarchy (2.16) associated to problem  $(\text{SQP}_M)$  is a closed set. Hence, the 'sup' in program (2.16) can be changed to a 'max'. As a consequence, for a matrix  $M \in \partial\text{COP}_n$ , having finite convergence of the Lasserre hierarchy (2.16) associated to problem  $(\text{SQP}_M)$  is equivalent to having  $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ . So we obtain the following corollary.

**Corollary 2.20.** *Let  $M \in \partial\text{COP}_n$ . If the optimality conditions (CQC), (SCC), and (SOSC) hold at every global minimizer of problem (SQP<sub>M</sub>), then  $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ .*

**2.4.1. Optimality conditions of problem (SQP<sub>M</sub>).** In this section, we give sufficient conditions on  $M$  that permit to claim  $DMD \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$  for all  $D \in \mathcal{D}_{++}^n$ . For this, we will apply Corollary 2.20, combined with the following result, which will be a key ingredient in our argument.

**Theorem 2.21.** *If the optimality conditions (CQC), (SCC), and (SOSC) hold at every minimizer of problem (SQP<sub>M</sub>) for a matrix  $M \in \partial\text{COP}_n$ , then, for every  $D \in \mathcal{D}_{++}^n$ , they also hold at every minimizer of problem (SQP<sub>DMD</sub>).*

In what follows we will prove Theorem 2.21. Given  $M \in \partial\text{COP}_n$  and  $D \in \mathcal{D}_{++}^n$ , let us consider the standard quadratic program associated to  $DMD$ :

$$\min\{x^T DMDx : x \in \Delta_n\}. \quad (\text{SQP}_{DMD})$$

Observe that  $DMD \in \partial\text{COP}_n$ , i.e., the optimal value of program (SQP<sub>DMD</sub>) is zero. Indeed, if  $u \in \Delta_n$  is a minimizer of problem (SQP<sub>M</sub>), then the vector  $\frac{D^{-1}u}{\|D^{-1}u\|_1} \in \Delta_n$  is a minimizer of problem (SQP<sub>DMD</sub>). Conversely, if  $v \in \Delta_n$  is a minimizer of (SQP<sub>DMD</sub>), then  $\frac{Dv}{\|Dv\|_1}$  is a minimizer of (SQP<sub>M</sub>). Hence, the minimizers of both problems are in one-to-one correspondence, and thus problem (SQP<sub>M</sub>) has finitely many minimizers if and only if problem (SQP<sub>DMD</sub>) has finitely many minimizers.

Now, we analyze the optimality conditions (CQC), (SCC), and (SOSC) for problems (SQP<sub>M</sub>) and (SQP<sub>DMD</sub>). Observe that the constraint qualification condition (CQC) is satisfied at every minimizer. Indeed, if  $u \in \Delta_n$ , then the set of inequalities that are active at  $u$  is  $J(u) = \{i \in [n] : x_i = 0\}$ , and the vectors  $e, e_i$  (for  $i \in J(u)$ ) are linearly independent. This last claim follows from the fact that  $J(u) \neq [n]$  as  $\sum_{i=1}^n x_i = 1$ .

Let us recall a result from [Dian62] about the support of optimal solutions for problem (SQP<sub>M</sub>), which we will use for the analysis of the conditions (SCC) and (SOSC). We give a short proof for clarity.

**Lemma 2.22.** [Dian62, Lemma 7 (i)] *Let  $M \in \text{COP}_n$  and let  $x \in \mathbb{R}_+^n$  be such that  $x^T Mx = 0$ . Let  $S = \text{Supp}(x)$  be the support of  $x$ . Then  $M[S]$ , the principal submatrix of  $M$  indexed by  $S$ , is positive semidefinite.*

PROOF. Let  $\tilde{x} = x|_S$  be the restriction of  $x$  to the coordinates indexed by  $S$ , so  $\tilde{x}^T M[S]\tilde{x} = 0$ . Assume by contradiction that  $M[S]$  is not positive semi-definite. Then there exists  $y \in \mathbb{R}^S$  such that  $y^T M[S]y < 0$  and we can assume that  $y^T M[S]\tilde{x} \leq 0$  (else replace  $y$  by  $-y$ ). Since all entries of  $\tilde{x}$  are positive, there exists  $\lambda \geq 0$  such that the vector  $\lambda\tilde{x} + y$  has all its entries positive. Thus,  $(\lambda\tilde{x} + y)^T M[S](\lambda\tilde{x} + y) = \lambda^2 \tilde{x}^T M[S]\tilde{x} + 2\lambda \tilde{x}^T M[S]y + y^T M[S]y < 0$ , contradicting that  $M[S]$  is copositive.  $\square$

We now characterize the minimizers for which the strict complementarity condition (SCC) holds. Moreover, we show that, if a minimizer  $u$  of problem  $(SQP_M)$  satisfies (SCC), then the corresponding minimizer  $\frac{D^{-1}u}{\|D^{-1}u\|}$  of problem  $(SQP_{DMD})$  also satisfies (SCC).

**Lemma 2.23.** *Let  $M \in \partial\text{COP}_n$ ,  $D \in \mathcal{D}_{++}^n$ , and let  $u$  be a minimizer of problem  $(SQP_M)$ . The strict complementarity condition (SCC) holds at  $u$  if and only if  $\text{Supp}(Mu) = [n] \setminus \text{Supp}(u)$  or, equivalently,  $(Mu)_i > 0$  for all  $i \in [n] \setminus \text{Supp}(u)$ .*

*As a consequence, (SCC) holds at  $u$  (for problem  $(SQP_M)$ ) if and only if (SCC) holds at  $\frac{D^{-1}u}{\|D^{-1}u\|}$  (for problem  $(SQP_{DMD})$ ).*

PROOF. Let  $S = \text{Supp}(u)$ . We first prove that  $(Mu)_i = 0$  for any  $i \in S$ . Let  $\tilde{u} = u|_S$  denote the restriction of vector  $u$  to the coordinates indexed by  $S$ . Then, we have  $0 = u^T Mu = \tilde{u}^T M[S]\tilde{u}$ . By Lemma 2.22,  $M[S]$  is positive semidefinite, and thus  $\tilde{u} \in \text{Ker}(M[S])$ . Thus,  $0 = (M[S]\tilde{u})_i = (Mu)_i$  for any  $i \in S$ . This shows  $\text{Supp}(Mu) \subseteq [n] \setminus S$ . Hence equality  $\text{Supp}(Mu) = [n] \setminus S$  holds if and only if  $(Mu)_i = \sum_{j \in \text{Supp}(u)} M_{ij}u_j > 0$  for all  $i \in [n] \setminus \text{Supp}(u)$ . It suffices now to show the link to (SCC).

In problem  $(SQP_M)$  the strict complementarity condition (SCC) reads:

$$Mu = \lambda e + \sum_{j \in [n] \setminus S} \mu_j e_j \quad \text{with } \mu_j > 0 \text{ for } j \in [n] \setminus S.$$

By looking at the coordinate indexed by  $i \in S$  we obtain that  $0 = (Mu)_i = \lambda$ . Hence,  $(Mu)_j = \mu_j$  for any  $j \in [n] \setminus S$ . Therefore (SCC) holds if and only if  $(Mu)_j > 0$  for all  $j \in [n] \setminus S$ .

The last claim of the lemma follows using the above characterization, combined with the correspondence between the minimizers  $u$  of  $(SQP_M)$  and  $D^{-1}u$  (up to scaling) of  $(SQP_{DMD})$  and the fact that  $\text{Supp}(Mu) = \text{Supp}(DMu)$  and  $\text{Supp}(D^{-1}u) = \text{Supp}(u)$  (as  $D$  is positive diagonal).  $\square$

As observed, e.g., in [Nie12], if the sufficient optimality conditions (CQC), (SCC), (SOSC) hold at every global minimizer, then the number of minimizers must be finite. We now show a useful fact: if a standard quadratic program has finitely many minimizers, then (SOSC) holds at all of them.

**Lemma 2.24.** *Let  $M \in \partial\text{COP}_n$ , so that problem  $(SQP_M)$  has optimal value zero. If  $(SQP_M)$  has finitely many minimizers, then (SOSC) holds at every global minimizer.*

PROOF. Assume  $M \in \partial\text{COP}_n$  and  $(SQP_M)$  has finitely many minimizers. We first prove that, given  $S \subseteq [n]$ , problem  $(SQP_M)$  has at most one optimal solution with support  $S$ . For this, assume by contradiction that  $u \neq v \in \Delta_n$  are solutions of  $x^T Mx = 0$  with support  $S$ . By Lemma 2.22 the matrix  $M[S]$  is positive semidefinite. Let  $\tilde{u}$  and  $\tilde{v}$  be the restrictions of the vectors  $u$  and  $v$  to the entries indexed by  $S$ . Hence,  $\tilde{u}^T M[S]\tilde{u} = \tilde{v}^T M[S]\tilde{v} = 0$ , and thus

$M[S]\tilde{u} = M[S]\tilde{v} = 0$ . This implies that every convex combination of  $\tilde{u}, \tilde{v}$  belongs to the kernel of  $M[S]$ , so that the form  $x^T M[S]x$  has infinitely many zeros on  $\Delta_{|S|}$ . Hence,  $x^T Mx$  has infinitely many zeros on  $\Delta_n$ , contradicting the assumption.

Let  $u$  be a minimizer of problem (SQP<sub>M</sub>) with support  $S$  and consider as above its restriction  $\tilde{u} \in \mathbb{R}^{|S|}$ . Observe that the *second order sufficiency condition* (SOSC) for problem (SQP<sub>M</sub>) at  $u$  reads

$$v^T Mv > 0 \text{ for all } v \in \mathbb{R}^n \setminus \{0\} \text{ such that } \sum_{i=1}^n v_i = 0 \text{ and } v_j = 0 \quad \forall j \in [n] \setminus S,$$

$$\text{or, equivalently, } a^T M[S]a > 0 \text{ for all } a \in \mathbb{R}^{|S|} \setminus \{0\} \text{ such that } \sum_{i \in S} a_i = 0.$$

Assume that  $a^T M[S]a = 0$ , we show  $a = 0$ . Since  $M[S] \succeq 0$  we have that  $M[S]a = 0$ , so that  $M[S](\lambda\tilde{u} + a) = 0$  for all  $\lambda \in \mathbb{R}$ . Pick  $\lambda > 0$  large enough so that all entries of  $\lambda\tilde{u} + a$  are positive. Then,  $\lambda\tilde{u} + a$  should be a multiple of  $\tilde{u}$  because  $u$  is the only minimizer over the simplex with support  $S$ . Combining with the fact that  $e^T a = 0$ , this implies  $a = 0$ .  $\square$

As previously observed, the minimizers of problems (SQP<sub>M</sub>) and (SQP<sub>DMD</sub>) are in one-to-one correspondence. Thus, as a consequence of Lemma 2.24, (SOSC) holds at every global minimizer of (SQP<sub>M</sub>) if and only if it holds at every global minimizer of problem (SQP<sub>DMD</sub>). Moreover, we have shown in Lemma 2.23 that (SCC) holds for all minimizers of problem (SQP<sub>DMD</sub>) if and only if it holds for all minimizers of (SQP<sub>M</sub>). Therefore, we have now completed the proof of Theorem 2.21. Moreover, combining Corollary 2.20 and the characterization of (SCC) in Lemma 2.23, we obtain the following result, useful for further reference.

**Theorem 2.25.** *Let  $M \in \partial\text{COP}_n$  and assume problem (SQP<sub>M</sub>) has finitely many minimizers. Assume moreover that, for every minimizer  $u$  of problem (SQP<sub>M</sub>), we have  $(Mu)_i > 0$  for all  $i \in [n] \setminus \text{Supp}(u)$ . Then we have*

$$DMD \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} \quad \text{for all } D \in \mathcal{D}_{++}^n.$$

The following example shows a copositive matrix  $M$  for which the form  $x^T Mx$  has a unique zero in  $\Delta_n$ ; however  $M$  does not belong to  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ , and thus it also does not belong to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$  (in view of relation (2.1)). Hence, the condition on the support of the zeros in Theorem 2.25 cannot be omitted.

**Example 2.26.** *Let  $M_1$  be a matrix lying in  $\text{int}(\text{COP}_n) \setminus \mathcal{K}_n^{(0)}$ . Such a matrix exists for any  $n \geq 5$ . As an example for  $M_1$ , one may take the Horn matrix  $H$  in (2.4), in which we replace all entries 1 by  $t$ , where  $t$  is a given scalar*

such that  $1 < t < \sqrt{5} - 1$  (see [LV22b]). By Theorem 2.7, we have

$$M := \left( \begin{array}{c|cc} M_1 & & 0 \\ \hline & 1 & -1 \\ 0 & -1 & 1 \end{array} \right) \in \text{COP}_{n+2} \setminus \bigcup_{r \geq 0} \mathcal{K}_{n+2}^{(r)}. \quad (2.18)$$

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  $x^T M x = 0$ . As  $M_1$  is strictly copositive (see e.g. [dKP02]) 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  $\Delta_2$  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  $\Delta_n$  is  $x = (0, 0, \dots, 0, \frac{1}{2}, \frac{1}{2})$ , as desired.

**2.4.2. Proof of Theorem 2.5.** Now, we can prove the result of Theorem 2.5; that is, we show that  $DT(\psi)D \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$  for all  $D \in \mathcal{D}_{++}^n$  and  $\psi \in \Psi$ . We show this result as an application of Theorem 2.25. It thus remains to check that the two assumptions in Theorem 2.25 hold. First, by combining two results from [Hil12], the description of the (finitely many) minimizers of problem  $(\text{SQP}_M)$  for  $M = T(\psi)$  ( $\psi \in \Psi$ ) can be found.

**Lemma 2.27.** *The minimizers of problem  $(\text{SQP}_M)$  associated to the matrix  $M = T(\psi)$  (with  $\psi \in \Psi$ ) are the vectors  $v_i = \frac{u_i}{\|u_i\|_1}$  for  $i \in [5]$ , where the  $u_i$ 's are defined by*

$$u_1 = \begin{pmatrix} \sin \psi_5 \\ \sin(\psi_4 + \psi_5) \\ \sin \psi_4 \\ 0 \\ 0 \end{pmatrix}, \quad u_2 = \begin{pmatrix} \sin(\psi_3 + \psi_4) \\ \sin \psi_3 \\ 0 \\ 0 \\ \sin \psi_4 \end{pmatrix}, \quad u_3 = \begin{pmatrix} 0 \\ \sin \psi_1 \\ \sin(\psi_1 + \psi_5) \\ \sin \psi_5 \\ 0 \end{pmatrix}, \quad u_4 = \begin{pmatrix} 0 \\ 0 \\ \sin \psi_2 \\ \sin(\psi_1 + \psi_2) \\ \sin \psi_1 \end{pmatrix}, \quad u_5 = \begin{pmatrix} \sin \psi_2 \\ 0 \\ 0 \\ \sin \psi_3 \\ \sin(\psi_2 + \psi_3) \end{pmatrix}.$$

PROOF. By [Hil12, Theorem 2.5]) it follows that there are exactly five minimizers and that they are supported, respectively, by the sets  $\{1, 2, 3\}$ ,  $\{1, 2, 5\}$ ,  $\{2, 3, 4\}$ ,  $\{3, 4, 5\}$  and  $\{1, 4, 5\}$ . Next, using [Hil12, Lemma 3.2]), we obtain that the minimizers take the desired form.  $\square$

We finally check that the second assumption of Theorem 2.25 holds for the matrices  $M = T(\psi)$  ( $\psi \in \Psi$ ).

**Lemma 2.28.** *Let  $\psi \in \Psi$  and let  $v$  be a minimizer of problem  $(\text{SQP}_M)$  where  $M = T(\psi)$ . Then, we have  $(Mv)_i > 0$  for all  $i \in [5] \setminus \text{Supp}(v)$ .*

PROOF. By symmetry, it is enough to check this condition for one of the minimizers, say  $v_1$  (as given in Lemma 2.27). Since multiplying by a positive constant does not affect the sign we verify the condition for the vector  $u_1$ . For convenience, we set  $u = u_1$ . As  $\text{Supp}(u) = \{1, 2, 3\}$ , the condition we want to check reads as follows

$$\sum_{i=1}^3 T(\psi)_{i4} u_i > 0 \quad \text{and} \quad \sum_{i=1}^3 T(\psi)_{i5} u_i > 0.$$

Again, it suffices to check just the first inequality since the second one is analogous (up to index permutation). We will now check that the first expression is positive. Indeed we have

$$\begin{aligned}
& \sum_{i=1}^3 T(\psi)_{i4} u_i \\
&= \cos(\psi_2 + \psi_3) \sin \psi_5 + \cos(\psi_5 + \psi_1) \sin(\psi_4 + \psi_5) - \cos \psi_1 \sin \psi_4 \\
&= \cos(\psi_2 + \psi_3) \sin \psi_5 \\
&\quad + (\cos \psi_5 \cos \psi_1 - \sin \psi_5 \sin \psi_1)(\sin \psi_4 \cos \psi_5 + \cos \psi_4 \sin \psi_5) - \cos \psi_1 \sin \psi_4 \\
&= \cos(\psi_2 + \psi_3) \sin \psi_5 + (\cos^2 \psi_5 - 1) \cos \psi_1 \sin \psi_4 + \cos \psi_5 \cos \psi_1 \cos \psi_4 \sin \psi_5 \\
&\quad - \sin \psi_5 \sin \psi_1 \sin \psi_4 \cos \psi_5 - \sin^2 \psi_5 \sin \psi_1 \cos \psi_4 \\
&= \cos(\psi_2 + \psi_3) \sin(\psi_5) - \sin^2 \psi_5 \sin(\psi_1 + \psi_4) + \sin \psi_5 \cos \psi_5 \cos(\psi_1 + \psi_4) \\
&= \cos(\psi_2 + \psi_3) \sin \psi_5 + \sin \psi_5 \cos(\psi_1 + \psi_4 + \psi_5) \\
&= \sin \psi_5 (\cos(\psi_2 + \psi_3) + \cos(\psi_1 + \psi_4 + \psi_5)).
\end{aligned}$$

We finish the proof by showing that both factors in the last expression are positive for  $\psi \in \Psi$ . By the definition of  $\Psi$ ,  $\sum_{i=1}^5 \psi_i < \pi$  and  $\psi_i > 0$  for  $i \in [5]$ , so that  $\psi_5 \in (0, \pi)$  and thus  $\sin \psi_5 > 0$ . Now, we use that cosine is a monotone decreasing function in the interval  $(0, \pi)$ . Observe that  $\psi_2 + \psi_3$  and  $\pi - (\psi_1 + \psi_4 + \psi_5)$  belong to  $(0, \pi)$  and  $\psi_2 + \psi_3 < \pi - (\psi_1 + \psi_4 + \psi_5)$ . Thus,  $\cos(\psi_2 + \psi_3) > \cos(\pi - (\psi_1 + \psi_4 + \psi_5)) = -\cos(\psi_1 + \psi_4 + \psi_5)$ , completing the proof.  $\square$

## CHAPTER 3

# Semidefinite approximations for the stability number

*This chapter provides background about different approaches based on semidefinite programming for bounding the stability number of a graph, that will be studied in the rest of this thesis. The results from Section 3.4.2 are new, unless otherwise specified.*

Given a graph  $G = (V, E)$ , recall that a subset  $S \subseteq V$  is stable if  $S$  contains no edge, i.e.,  $\{i, j\} \notin E$  for any pair of nodes  $i, j \in S$ . Recall also that the stability number of  $G$ , denoted by  $\alpha(G)$ , is the maximum cardinality of a stable set in  $G$ . We say that a set is  $\alpha$ -stable if it is stable with cardinality  $\alpha(G)$ . As mentioned in the introduction, computing  $\alpha(G)$  is well-known to be NP-hard [Kar72]. In this section, we recall some approaches for approximating  $\alpha(G)$  via semidefinite programming. We give special attention to the upper bounds  $\vartheta^{(r)}(G)$  introduced by de Klerk and Pasechnik in [dKP02] (see Section 3.4).

### 3.1. Lovász $\vartheta$ -number

The Lovász  $\vartheta$ -number was defined by Lovász in his seminal paper [Lov79] with the goal of estimating the Shannon capacity of a graph. There are many ways for defining  $\vartheta(G)$  (see, for example, the survey [Knuth94]). We recall one of its definitions:

$$\vartheta(G) := \max_{X \in \mathcal{S}^n} \{ \langle J, X \rangle : X_{ij} = 0 \text{ for } \{i, j\} \in E, \text{Tr}(X) = 1, X \succeq 0 \}. \quad (3.1)$$

From the definition it is easy to observe that

$$\alpha(G) \leq \vartheta(G).$$

Indeed, if  $S$  is a stable set of size  $\alpha(G)$ , then the matrix  $X = \frac{1}{\alpha(G)} \chi^S (\chi^S)^\top$  is feasible for program (3.1) with value  $\alpha(G)$ , where  $\chi^S \in \mathbb{R}^V$  is the indicator vector of  $S$ .

The *clique covering number* of  $G$ , denoted by  $\bar{\chi}(G)$ , is the minimum number of cliques in  $G$  needed to cover  $V$ . In other words,  $\bar{\chi}(G)$  is the chromatic number of the graph  $\bar{G}$ , so  $\bar{\chi}(G) = \chi(\bar{G})$ . We have that  $\alpha(G) \leq \bar{\chi}(G)$  since a clique cannot contain two vertices from an independent set. This inequality

can be strict. For example, for the 5-cycle  $G = C_5$  we have  $\alpha(G) = 2$  while  $\bar{\chi}(G) = 3$ .

Lovász showed that the parameter  $\vartheta(G)$  lies in-between  $\alpha(G)$  and  $\bar{\chi}(G)$ .

**Lemma 3.1** (Sandwich Lemma [Lov79]). *Let  $G$  be a graph. We have*

$$\alpha(G) \leq \vartheta(G) \leq \bar{\chi}(G).$$

A graph  $G$  is called *perfect* if the equality  $\alpha(H) = \bar{\chi}(H)$  holds for all induced subgraph  $H$  of  $G$ . From Lemma 3.1, it follows that for any perfect graph  $\alpha(G) = \vartheta(G)$ , and thus  $\alpha(G)$  can be computed in polynomial time for perfect graphs (by computing  $\vartheta(G)$  with accuracy  $\frac{1}{4}$ ). Moreover, it was shown by Grötschel, Lovász and Schrijver in [GLS93] that one can also find a maximum stable set and a minimum coloring in perfect graphs in polynomial time using the parameter  $\vartheta(G)$ . A strengthening of  $\vartheta(G)$  was proposed by Schrijver in [Schr79] (see also [Mc79] for an equivalent definition) by restricting program (3.1) to matrices with nonnegative entries:

$$\vartheta'(G) := \max_{X \in \mathcal{S}^n} \{ \langle J, X \rangle : X_{ij} = 0 \text{ for } \{i, j\} \in E, \text{Tr}(X) = 1, X \succeq 0, X \geq 0 \}. \quad (3.2)$$

Then, we have

$$\alpha(G) \leq \vartheta'(G) \leq \vartheta(G) \leq \chi(\bar{G}). \quad (3.3)$$

The inequality  $\vartheta'(G) \leq \vartheta(G)$  can be strict. For example, when  $G$  is the graph with vertex set  $\{0, 1\}^6$  and two vectors are adjacent if their Hamming distance is at most 3. As pointed out in [Schr79], it was shown by M.R. Best that for this graph we have  $4 = \alpha(G) = \vartheta'(G) < \vartheta(G) = \frac{16}{3}$ .

### 3.2. Polynomial optimization formulations

In this section, we present some formulations for  $\alpha(G)$  as instance of polynomial optimization problems. Then, we will consider approximation hierarchies based on sums of squares of polynomials.

**3.2.1. Discrete formulation.** The first formulation arises naturally by considering the 0-1 formulation for  $\alpha(G)$ :

$$\alpha(G) = \max \left\{ \sum_{i=1}^n x_i : x_i x_j = 0 \text{ for } \{i, j\} \in E, x_i^2 - x_i = 0 \text{ for } i \in V \right\}. \quad (3.4)$$

We can now consider the corresponding Lasserre sum-of-squares hierarchy for (3.4). We first define the graph ideal given by the graph  $G$ :

$$I_G := I \left( \{x_i - x_i^2 : i \in V\} \cup \{x_i x_j : \{i, j\} \in E\} \right), \quad (3.5)$$



and the corresponding  $2r$ -truncated graph ideal given by  $G$ :

$$I_{2r,G} := I\left(\{x_i - x_i^2 : i \in V\} \cup \{x_i x_j : \{i, j\} \in E\}\right)_{2r}. \quad (3.6)$$

So, the Lasserre hierarchy for problem (3.4) reads

$$\text{las}_r(G) = \min\left\{\lambda : \lambda - \sum_{i=1}^n x_i \in \Sigma_{2r} + I_{2r,G}\right\}. \quad (3.7)$$

As is well-known (see, for example, Chapter 7) the level  $r = 1$  of the hierarchy (3.7) corresponds to  $\vartheta(G)$ , i.e.,

$$\text{las}_1(G) = \vartheta(G).$$

Also, it is known that the hierarchy  $\text{las}_r(G)$  converges to  $\alpha(G)$  after  $\alpha(G)$  steps (see, for example [Lau03]).

**Theorem 3.2.** *Let  $G$  be a graph. Then,  $\text{las}_{\alpha(G)}(G) = \alpha(G)$ .*

This last result follows from the following more general fact (see [Las01a] and [Lau03]):

$$p \geq 0 \text{ on } \left\{x \in \mathbb{R}^V : x_i - x_i^2 = 0 \text{ for } i \in V, x_i x_j = 0 \text{ for } \{i, j\} \in E\right\} \quad (3.8)$$

$$\iff p \in \Sigma_{\alpha(G)} + I_G.$$

Gvozdenović and Laurent [GL07] consider the following strengthening of the hierarchy  $\text{las}_r(G)$ :

$$\text{las}^{(r)}(G) = \min\left\{\lambda : \lambda - \sum_{i=1}^n x_i = \sigma + p + \sum_{\substack{I \subset [n] \\ |I|=r+1}} a_I x^I, \quad (3.9)$$

$$\text{where } \sigma \in \Sigma_{2r}, p \in I_{2r,G}, a_I \geq 0\right\}.$$

Hence,  $\alpha(G) \leq \text{las}^{(r)}(G) \leq \text{las}_r(G)$  and thus, in view of Theorem 3.2, we have  $\text{las}^{(\alpha(G))}(G) = \alpha(G)$ . It was shown in [GL07] that the level  $r = 1$  corresponds to the bound  $\vartheta'(G)$ :

$$\text{las}^{(1)}(G) = \vartheta'(G).$$

**3.2.2. Continuous formulation.** Another starting point for defining hierarchies of approximations for the stability number is the following formulation by Motzkin and Straus [MS65], which expresses  $\frac{1}{\alpha(G)}$  via quadratic optimization over the standard simplex  $\Delta_n$ .

**Theorem 3.3** ([MS65]). *Let  $G = ([n], E)$  be a graph with stability number  $\alpha(G)$ . Then, we have*

$$\frac{1}{\alpha(G)} = \min\left\{x^T(A_G + I)x : x \in \Delta_n\right\}. \quad (\text{M-S})$$

Here,  $A_G$  is the adjacency matrix of  $G$ . i.e.,  $A_G \in \mathcal{S}^n$ ,  $(A_G)_{ij} = 1$  if  $\{i, j\} \in E$  and  $(A_G)_{ij} = 0$  if  $\{i, j\} \notin E$ .

Let  $\chi^S \in \mathbb{R}^n$  be the indicator vector of the set  $S$ , i.e.,  $(\chi^S)_i = 1$  for  $i \in S$  and  $(\chi^S)_i = 0$  for  $i \notin S$ . Observe that for any  $\alpha$ -stable set  $S$  of  $G$  the vector  $x = \frac{\chi^S}{\alpha(G)}$  is a minimizer of problem (M-S). In general, these are not the only minimizers. The minimizers of (M-S) are fully characterized in Chapter 4 and this characterization will be crucial for the analysis of the convergence of the corresponding Lasserre hierarchy for problem (M-S).

It turns out that the formulation (M-S) (and some variations of it) provides a rich playground for analyzing complexity aspects of polynomial optimization problems and their Lasserre hierarchies. Indeed, in Chapter 4, we will use a perturbation of program (M-S) for showing that it is NP-hard to decide whether a standard quadratic program has finitely many minimizers, and that it is NP-hard to decide whether the Lasserre hierarchy of a polynomial optimization problem has finite convergence.

### 3.3. Copositive formulation

In this section, we focus on the hierarchies of approximations that naturally arise when considering the following copositive reformulation for  $\alpha(G)$ , given by de Klerk and Pasechnik [dKP02]:

$$\alpha(G) = \min\{t : t(I + A_G) - J \in \text{COP}_n\}. \quad (3.10)$$

Recall that  $A_G, I$ , and  $J$  are, respectively, the adjacency matrix of  $G$ , the identity, and the all-ones matrix. As a consequence, it follows from (3.10) that the following *graph matrix*

$$M_G := \alpha(G)(I + A_G) - J \quad (3.11)$$

belongs to  $\text{COP}_n$ . The copositive reformulation (3.10) for  $\alpha(G)$  can be seen as an application of the quadratic formulation by Motzkin and Straus shown in (M-S). Indeed, it is easy to observe that if  $t$  is feasible for (3.10), then the diagonal entries of  $t(A_G + I) - J$  are nonnegative and thus  $t \geq 1$ . Then, we have:

$$\begin{aligned} & t(A_G + I) - J \in \text{COP}_n \\ \iff & x^T(t(A_G + I) - J)x \geq 0 && \forall x \in \Delta_n \\ \iff & tx^T(A_G + I)x - 1 \geq 0 && \forall x \in \Delta_n \\ \iff & x^T(A_G + I)x \geq \frac{1}{t} && \forall x \in \Delta_n. \end{aligned}$$

Using the result of Theorem 3.3, we obtain that the optimal value of program (3.10) is  $\alpha(G)$ , as desired.

De Klerk and Pasechnik proposed two hierarchies of approximations using the cones  $\mathcal{C}_n^{(r)}$  and  $\mathcal{K}_n^{(r)}$  defined in relations (1.20) and (1.21). For clarity, we

recall the definition of these cones:

$$\mathcal{C}_n^{(r)} = \left\{ M : \left( \sum_{i=1}^n x_i \right)^r x^\top M x \in \mathbb{R}_+[x] \right\},$$

$$\mathcal{K}_n^{(r)} = \left\{ M : \left( \sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^\top M x^{\circ 2} \in \Sigma \right\}.$$

**The hierarchy  $\zeta^{(r)}(G)$ .** The parameters  $\zeta^{(r)}(G)$  were defined by replacing the cone  $\text{COP}_n$  by  $\mathcal{C}_n^{(r)}$  in problem (3.10). Then, for an integer  $r \geq 0$ , we have

$$\zeta^{(r)}(G) := \min\{t : t(A_G + I) - J \in \mathcal{C}_n^{(r)}\}. \quad (3.12)$$

Since  $\text{int}(\text{COP}_n) \subseteq \bigcup_{r>0} \mathcal{C}_n^{(r)}$ , it follows directly that the parameters  $\zeta^{(r)}(G)$  converge asymptotically to  $\alpha(G)$  as  $r \rightarrow \infty$ . Note that, if  $G = K_n$  is a complete graph, then  $\alpha(G) = 1$  and the matrix  $I + A_G - J$  is the zero matrix, thus belonging trivially to the cone  $\mathcal{C}_n^{(0)}$ , so that  $1 = \alpha(K_n) = \zeta^{(0)}(K_n)$ . However, finite convergence does not hold if  $G$  is not a complete graph.

**Theorem 3.4** (de Klerk, Pasechnik [dKP02]). *Assume  $G$  is not a complete graph. Then, we have  $\zeta^{(r)}(G) > \alpha(G)$  for all  $r \in \mathbb{N}$ .*

By the definition of the cone  $\mathcal{C}_n^{(r)}$ , the parameter  $\zeta^{(r)}(G)$  can be formulated as a linear program, asking for the smallest scalar  $t$  for which all the coefficients of the polynomial  $(\sum_{i=1}^n x_i)^r x^\top (t(I + A_G) - J)x$  are nonnegative. The parameter  $\zeta^{(r)}(G)$  is very well understood. Indeed, Peña, Vera and Zuluaga [PVZ07] give a closed-form expression for it in terms of  $\alpha(G)$ .

**Theorem 3.5** (Peña, Vera, Zuluaga [PVZ07]). *Write  $r + 2 = u\alpha(G) + v$ , where  $u, v$  are nonnegative integers such that  $v \leq \alpha(G) - 1$ . Then we have*

$$\zeta^{(r)}(G) = \frac{\binom{r+2}{2}}{\binom{u}{2}\alpha(G) + uv},$$

where we set  $\zeta^{(r)}(G) = \infty$  if  $r \leq \alpha(G) - 2$  (since then the denominator in the above formula is equal to 0).

A consequence of this result is that after  $r = \alpha(G)^2 - 1$  steps we find  $\alpha(G)$  up to rounding. (See also [dKP02] where this result is shown for  $r = \alpha(G)^2$ ).

**Corollary 3.6** ([PVZ07]). *We have equality  $\lfloor \zeta^{(r)}(G) \rfloor = \alpha(G)$  if and only if  $r \geq \alpha(G)^2 - 1$ .*

### 3.4. The hierarchy $\vartheta^{(r)}(G)$

We now dedicate a separate section to the parameters  $\vartheta^{(r)}(G)$ , for  $r \in \mathbb{N}$ , which play a central role in this thesis. In this section, we will give the basic

definitions and facts that will be used in Chapters 4, 5 and 6. The hierarchy  $\vartheta^{(r)}(G)$  was defined as follows in [dKP02]:

$$\vartheta^{(r)}(G) := \min\{t : t(A_G + I) - J \in \mathcal{K}_n^{(r)}\}. \quad (3.13)$$

Since  $\mathcal{C}_n^{(r)} \subseteq \mathcal{K}_n^{(r)} \subseteq \text{COP}_n$  we have  $\alpha(G) \leq \vartheta^{(r)}(G) \leq \zeta^{(r)}(G)$  for any  $r \geq 0$ , and thus the parameters  $\vartheta^{(r)}(G)$  converge asymptotically to  $\alpha(G)$  as  $r \rightarrow \infty$ .

At order  $r = 0$ , while  $\zeta^{(0)}(G) = \infty$ , the parameter  $\vartheta^{(0)}(G)$  provides a useful bound for  $\alpha(G)$ . Indeed, it is shown in [dKP02] that  $\vartheta^{(0)}(G)$  coincides with  $\vartheta'(G)$  defined in at the beginning of this section. So, we have the inequalities

$$\alpha(G) \leq \vartheta'(G) = \vartheta^{(0)}(G) \leq \vartheta(G).$$

This connection in fact motivates the choice of the notation  $\vartheta^{(r)}(G)$ .

**3.4.1. Convergence properties of  $\vartheta^{(r)}$  and conjecture.** In Theorem 3.4, we saw that the bounds  $\zeta^{(r)}(G)$  are never exact unless  $G$  is a complete graph. This naturally raises the question of whether the (stronger) bounds  $\vartheta^{(r)}(G)$  may be exact. Recall the definition of the graph matrix  $M_G = \alpha(G)(A_G + I) - J$  in (3.11), and define the following polynomials

$$q_G := x^\top M_G x. \quad (3.14)$$

$$f_G := q_G(x^{\circ 2}) = (x^{\circ 2})^\top M_G x^{\circ 2}. \quad (3.15)$$

Then, for any  $r \in \mathbb{N}$ , we have

$$\vartheta^{(r)}(G) = \alpha(G) \iff M_G \in \mathcal{K}_n^{(r)} \iff \left( \sum_{i=1}^n x_i^2 \right)^r f_G \in \Sigma. \quad (3.16)$$

As  $M_G$  is copositive, the polynomial  $f_G$  is globally nonnegative. The point, however, is that  $f_G$  has zeros in  $\mathbb{R}^n \setminus \{0\}$ . In particular, for every stable set  $S \subseteq V$  of cardinality  $\alpha(G)$ , the indicator vector of  $S$ , denoted by  $\chi^S$ , is a zero of  $f_G$ . Thus, the question of whether  $f_G$  admits a positivity certificate of the form  $(\sum_{i=1}^n x_i^2)^r f_G \in \Sigma$  for some  $r \in \mathbb{N}$  (as in (1.8)) is nontrivial. In [dKP02] it was in fact conjectured that such a certificate exists at order  $r = \alpha(G) - 1$ ; in other words, that the parameter  $\vartheta^{(r)}(G)$  is exact at order  $r = \alpha(G) - 1$ .

**Conjecture 3.7** (de Klerk and Pasechnik [dKP02]). *For any graph  $G$ , we have  $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$ , or, equivalently, we have  $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$ .*

In relation (3.9) we introduced the parameters  $\text{las}^{(r)}(G)$ . In [GL07] it is shown that, for any integer  $r \geq 1$ , we have  $\alpha(G) \leq \text{las}^{(r)}(G) \leq \vartheta^{(r)}(G)$ . As mentioned before, the bounds  $\text{las}^{(r)}(G)$  are known to converge to  $\alpha(G)$  in  $\alpha(G)$  steps, i.e.,  $\text{las}^{(\alpha(G))}(G) = \alpha(G)$ . Thus, Conjecture 3.7 asks whether a similar

property holds for the parameters  $\vartheta^{(r)}(G)$ . While the finite convergence property for the Lasserre-type bounds is relatively easy to prove (by exploiting the fact that one works modulo the ideal generated by  $x_i^2 - x_i$  for  $i \in V$  and  $x_i x_j$  for  $\{i, j\} \in E$ ), proving Conjecture 3.7 seems much more challenging.

Conjecture 3.7 is known to hold for some graph classes. For instance, we saw above that it holds for perfect graphs (with  $r = 0$ ), but it also holds for odd cycles and their complements – that are not perfect (with  $r = 1$ , see [dKP02]). In [GL07], Conjecture 3.7 was shown to hold for all graphs  $G$  with  $\alpha(G) \leq 8$  (see also [PVZ07] for the case  $\alpha(G) \leq 6$ ). In fact, a stronger result is shown there: the proof relies on a technical construction of matrices that permit to certify membership of  $M_G$  in the cones  $\mathcal{Q}_n^{(r)}$  (and thus in the cones  $\mathcal{K}_n^{(r)}$ ). Whether Conjecture 3.7 holds in general is still an open problem. However, a weaker form of it is shown in this thesis; namely we show finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  to  $\alpha(G)$ , or, equivalently, membership of the graph matrices  $M_G$  in  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ . This result will be shown in Chapter 6.

**Theorem 3.8.** *Let  $G$  be a graph. Then, there exists  $r \in \mathbb{N}$  such that  $\vartheta^{(r)}(G) = \alpha(G)$ .*

**3.4.2.  $\vartheta$ -rank and simple graph operations.** We define the  $\vartheta$ -rank of  $G$  as the number of steps that the hierarchy  $\vartheta^{(r)}(G)$  takes to converge to  $\alpha(G)$ .

**Definition 3.9.** *Let  $G$  be a graph. We define the  $\vartheta$ -rank of  $G$  as*

$$\vartheta\text{-rank}(G) = \min\{r \in \mathbb{N} : \vartheta^{(r)}(G) = \alpha(G)\}.$$

*We set  $\vartheta\text{-rank}(G) = \infty$  if such  $r$  does not exist.*

In this section we discuss the behavior of the  $\vartheta$ -rank under simple graph operations: deleting a node belonging to a twin pair, deleting non-critical edges, and adding isolated nodes. The last two operations will be analyzed in more detail in Chapter 5.

**Twin pairs.** A pair of distinct nodes  $(u, v)$  is called a *twin pair* if  $\{u, v\} \in E$  and  $N_G(u) = N_G(v)$ . It is clear that if  $(u, v)$  is a twin pair, then  $\alpha(G) = \alpha(G \setminus u)$ . We show that the  $\vartheta$ -rank is invariant under deleting a node that belongs to a twin pair. Moreover, we show that membership of  $M_G$  in the cones  $\text{LAS}_{\Delta_n}^{(r)}$  is also invariant under this operation. The first part of this result (relation (3.17)) was already shown in [GL07].

**Lemma 3.10.** *Let  $G = ([n], E)$  be a graph. Assume  $(u, v)$  is a twin pair. Then, the following two equivalences hold.*

$$M_G \in \mathcal{K}_n^{(r)} \iff M_{G \setminus u} \in \mathcal{K}_{n-1}^{(r)}, \quad (3.17)$$

$$M_G \in \text{LAS}_{\Delta_n}^{(r)} \iff M_{G \setminus u} \in \text{LAS}_{\Delta_{n-1}}^{(r)}. \quad (3.18)$$

PROOF. Assume  $(u, v) = (1, 2)$ . The implications ‘ $\implies$ ’ in both relations (3.17) and (3.18) follow directly by setting  $x_1 = 0$  in any of the definitions of the cones  $\mathcal{K}_n^{(r)}$  and  $\text{LAS}_{\Delta_n}^{(r)}$  (e.g., (1.21) and (1.28)). For the reverse implications ‘ $\impliedby$ ’, we first observe that the following relation holds:

$$q_G(x_1, x_2, x_3, \dots, x_n) = q_{G \setminus 1}(x_1 + x_2, x_3, \dots, x_n). \quad (3.19)$$

(Recall the definition of  $q_G$  in (3.14)). First, assume that  $M_{G \setminus 1} \in \mathcal{K}_{n-1}^{(r)}$ . Then, using relation (1.24) for defining the cone  $\mathcal{K}_{n-1}^{(r)}$ , we have

$$\left( \sum_{i=2}^n x_i \right)^r q_{G \setminus 1}(x_2, \dots, x_n) = \sum_{\substack{\beta \in \mathbb{N}^{n-1} \\ |\beta| \leq r+2}} \sigma_\beta x^\beta \quad \text{for some } \sigma_\beta \in \Sigma_{r+2-|\beta|}.$$

By replacing  $x_2$  by  $x_1 + x_2$ , and using relation (3.19), we obtain

$$\left( \sum_{i=1}^n x_i \right)^r q_G(x_1, \dots, x_n) = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| \leq r+2}} \tilde{\sigma}_\beta x^\beta \quad \text{for some } \tilde{\sigma}_\beta \in \Sigma_{r+2-|\beta|},$$

showing that  $M_G \in \mathcal{K}_n^{(r)}$ .

Finally, assume  $M_{G \setminus 1} \in \text{LAS}_{\Delta_{n-1}}^{(r)}$ . Then, using definition (1.28) for  $\text{LAS}_{\Delta_{n-1}}^{(r)}$ ,

$$q_{G \setminus 1}(x_2, \dots, x_n) = \sigma_0 + \sum_{i=2}^n \sigma_i x_i + q \cdot \left( \sum_{i=2}^n x_i - 1 \right)$$

for  $\sigma_0 \in \Sigma_r, \sigma_i \in \Sigma_{r-1}, q \in \mathbb{R}[x_2, x_3, \dots, x_n]$ . Again, replacing  $x_2$  by  $x_1 + x_2$  and using relation (3.19), we obtain

$$q_G(x_1, \dots, x_n) = \tilde{\sigma}_0 + (x_1 + x_2)\tilde{\sigma}_2 + \sum_{i=3}^n \tilde{\sigma}_i x_i + \tilde{q} \cdot \left( \sum_{i=1}^n x_i - 1 \right),$$

for some  $\tilde{\sigma}_0 \in \Sigma_r, \tilde{\sigma}_i \in \Sigma_{r-1}, \tilde{q} \in \mathbb{R}[x]$ . This shows  $M_G \in \text{LAS}_{\Delta_n}^{(r)}$ .  $\square$

**Critical edges.** One notion that is going to be crucial throughout is the criticality of edges and graphs.

**Definition 3.11.** *Let  $G = (V, E)$  be a graph. An edge  $e \in E$  is called  $\alpha$ -critical (or, simply, critical) if  $\alpha(G \setminus e) = \alpha(G) + 1$ . We say that  $G$  is  $\alpha$ -critical (or, simply, critical) if all its edges are critical. We say that  $G$  is acritical if no edge of  $G$  is critical.*

We now make an observation about the structure of the critical edges. Recall that the symmetric difference of two sets  $A$  and  $B$ , denoted by  $A \triangle B$ , is defined as  $(A \cup B) \setminus (A \cap B)$ .

**Observation 3.12.** *An edge  $\{u, v\}$  is critical if and only if there exists  $I \subseteq V$  such that  $I \cup \{u\}$  and  $I \cup \{v\}$  are maximum stable sets in  $G$ . Hence, a graph is acritical if and only if, for any pair of maximum stable sets  $S_1$  and  $S_2$ , we have that  $|S_1 \Delta S_2| \geq 4$ .*

Notice that odd cycles are  $\alpha$ -critical graphs while even cycles are acritical. Critical edges and critical graphs have been studied in the literature; see, e.g. [LP86]. It turns out that the notion of critical edges plays a central role in the study of the convergence of the above hierarchies of bounds.

On the one hand, it can be easily observed that deleting noncritical edges can only increase the  $\vartheta$ -rank (see Lemma 5.10). Hence, after iteratively deleting noncritical edges, we obtain a subgraph  $H$  of  $G$ , which is critical with  $\alpha(H) = \alpha(G)$  and satisfies:  $\vartheta\text{-rank}(G) \leq \vartheta\text{-rank}(H)$ . Therefore, finite convergence of the parameters  $\vartheta^{(r)}(G)$  for the class of *critical* graphs implies the same property for general graphs. Analogously, it would suffice to show Conjecture 3.7 for the class of *critical* graphs.

On the other hand, as we will see in Chapter 4, we show that, for acritical graphs, the matrix  $M_G$  belongs to some cone  $\text{LAS}_{\Delta_n}^{(r)}$  (see Theorem 4.14). This implies, in particular, finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  for the class of acritical graphs, in view Theorem 2.10 and relation (3.16). A crucial point for showing this result is that the number of zeros of  $x^T M_G x$  in  $\Delta_n$  (or, equivalently, the number of minimizers of problem (M-S)) is finite precisely when  $G$  is acritical (see Theorem 4.11).

The notion of critical edges plays also a crucial role in the analysis of the graphs with  $\vartheta$ -rank 0 and 1. In Chapter 5, we can indeed characterize the *critical* graphs with  $\vartheta$ -rank 0. Namely, the graphs that are disjoint union of cliques. In addition, we show that the problem of deciding whether a graph has  $\vartheta$ -rank 0 can be algorithmically reduced to the same question restricted to the class of acritical graphs (see Theorem 5.38).

Papadimitriou and Wolfe [PW88] showed that given a graph  $G$  and an integer  $k$ , the problem of deciding whether  $G$  is critical with stability number  $k$  is DP-complete. The complexity class DP was introduced by Papadimitriou and Yannakakis [PY84] as the languages that can be obtained as intersection of a language in NP and a language in co-NP. In this thesis, we show that the problem of deciding whether an edge is critical in a graph is NP-hard (see Theorem 4.24) and the problem of computing the stability number for acritical graphs is also NP-hard (see Theorem 4.28).

**Isolated nodes.** The graph  $G \oplus i$  is the graph obtained by adding the isolated node  $i$  to the graph  $G$ . Understanding the relation between  $\vartheta\text{-rank}(G)$  and  $\vartheta\text{-rank}(G \oplus i)$  is surprisingly hard, and this is one of the main difficulties for attacking Conjecture 3.7. It was shown in [GL07] that Conjecture 3.7 holds if the  $\vartheta$ -rank does not increase when adding isolated nodes, i.e., if we have  $\vartheta\text{-rank}(G \oplus i) \leq \vartheta\text{-rank}(G)$  for all graphs  $G$ . However, in Chapter 5, we find

counterexamples for this last assertion. For example, if  $G$  is the graph obtained by adding 8 isolated nodes to  $C_5$ , then  $\vartheta\text{-rank}(G) = 1$ , but  $\vartheta\text{-rank}(G \oplus i) \geq 2$  (see Corollary 5.56).

In Chapter 5, we show that a weaker version of this refuted assertion implies the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ . Namely, if  $\vartheta\text{-rank}(G)$  remains finite when adding isolated nodes, then the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence for all graphs  $G$  (see Proposition 5.19). Finally, in Chapter 6, we use this reduction to prove the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ .



## Simplex-based approximations for $\alpha(G)$

*This chapter is mainly based on my work [LV22a] with Monique Laurent. Here, we adopt the notation from our works [LV22c] and [VL23]. This chapter also includes several results that are not yet published. In particular:*

- *Theorem 4.17 in Section 4.4, characterizing the graphs for which the simplex-based Lasserre hierarchy  $p_G^{(r)}$  has finite convergence.*
- *Corollary 4.27 in Section 4.5, showing that it is NP-hard to decide whether the Lasserre sum-of-squares hierarchy of a polynomial optimization problem has finite convergence.*
- *Proposition 4.28 in Section 4.5, showing that it is NP-hard to find the stability number for acritical graphs.*

### 4.1. Introduction

In this chapter, we analyze the hierarchy  $p_G^{(r)}$  ( $r \in \mathbb{N}$ ) arising as the Lasserre hierarchy of problem (M-S) (introduced in Section 3.2.2), thus defined as

$$p_G^{(r)} := \max \left\{ \lambda : x^\top (A_G + I)x - \lambda \in \mathcal{M}(\mathbf{x})_{2r} + I_{\Delta_n} \right\}. \quad (4.1)$$

A motivation for studying the bound  $p_G^{(r)}$  is that it can be linked to the parameter  $\vartheta^{(r)}(G)$  as follows (see Corollary 4.7): for any integer  $r \geq 0$ ,

$$\frac{1}{\alpha(G)} \geq \frac{1}{\vartheta^{(2r)}(G)} \geq p_G^{(r+1)}. \quad (4.2)$$

Therefore, the finite convergence of the hierarchy  $p_G^{(r)}$  (to  $\frac{1}{\alpha(G)}$ ) would imply the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  (to  $\alpha(G)$ ), which is one of the central questions of this thesis. It has been observed (e.g., in Section 3.4) that showing finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  is equivalent to showing that  $M_G$  belongs to some cone  $\mathcal{K}_n^{(r)}$ . For the parameters  $p_G^{(r)}$ , a similar relation holds: The hierarchy  $p_G^{(r)}$  has finite convergence if and only if  $M_G$  belongs to some cone  $\text{LAS}_{\Delta_n}^{(r)}$  (see relation (4.4)). The main result of this chapter is a characterization of the graphs for which the hierarchy  $p_G^{(r)}$  has finite convergence: if  $G$  does not have twin pairs, then  $p_G^{(r)}$  has finite convergence if and only if  $G$  is acritical (see Theorem 4.14). Notice that the presence of twin pairs

does not affect the finite convergence of the hierarchy  $p_G^{(r)}$ , as it was observed earlier in Lemma 3.10.

We observe that the bound  $p_G^{(r)}$  can be rewritten as follows, using the definition of the cones  $\text{LAS}_{\Delta_n}^{(r)}$  (see Section 4.2 for a complete exposition),

$$p_G^{(r)} = \max \left\{ \lambda : A_G + I - \lambda J \in \text{LAS}_{\Delta_n}^{(2r)} \right\}. \quad (4.3)$$

Hence, the following holds:

$$p_G^{(r)} \text{ has finite convergence} \iff M_G \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}. \quad (4.4)$$

Recall that  $M_G = \alpha(G)(A_G + I) - J$  lies in the boundary of the copositive cone. Our approach relies on applying the result of Theorem 2.25, where we developed sufficient conditions for showing that a copositive matrix  $M \in \partial\text{COP}_n$  belongs to some cone  $\text{LAS}_{\Delta_n}^{(r)}$ . One restriction of this result is that it can only be applied when problem  $(\text{SQP}_M)$  has finitely many minimizers. We will see that, for the matrix  $M_G$ , this is precisely the case when  $G$  is acritical. This is the central topic of Section 4.3, where we characterize the minimizers of the Motzkin-Straus formulation in the more general setting of the weighted stable set problem. Observe that the minimizers of (M-S) are precisely the zeros of the form  $x^T M_G x$  on  $\Delta_n$ .

**Number of global minimizers and finite convergence.** A main reason why critical edges play a role in the study of finite convergence comes from the fact that problem (M-S) has infinitely many global minimizers when  $G$  has critical edges. Indeed, next to the global minimizers arising from the maximum stable sets (of the form  $\chi^S/\alpha(G)$  with  $S$  stable of size  $\alpha(G)$ ), also some special convex combinations of them are global minimizers when  $G$  has critical edges (see Corollary 4.12). Note that the existence of spurious minimizers (i.e., not directly arising from maximum stable sets) is well-known, see, e.g., [Bom97, PJ96]. Our approach to prove finite convergence of the bounds  $p_G^{(r)}$  is to apply Theorem 2.25, which is based on Nie's theorem (Theorem 1.13), and requires to check whether the classical sufficient optimality conditions hold at all global minimizers of (M-S). These conditions imply, in particular, that the problem must have finitely many minimizers, which explains why we can only apply it to acritical graphs.

There is a well-known easy remedy to force having finitely many minimizers, simply by perturbing the Motzkin-Straus formulation (M-S). Indeed, if we replace the adjacency matrix  $A_G$  by  $(1 + \varepsilon)A_G$  for any  $\varepsilon > 0$ , then the corresponding standard quadratic program still has optimal value  $1/\alpha(G)$ , but now the only global minimizers are those arising from the maximum stable sets. To get this property it would suffice to perturb the adjacency matrix at the positions corresponding to the critical edges of  $G$ . For the hierarchies of parameters obtained via this perturbed formulation, we can show the finite

convergence property, see Theorem 4.15 (which applies to the general setting of weighted graphs as discussed below). However, since we do not know a bound on the order of convergence, which *does not depend on*  $\varepsilon$ , it remains unclear how this can be used to derive the finite convergence of the original (unperturbed) parameters.

As a byproduct of our analysis of the minimizers of the (perturbed) Motzkin-Straus formulation, we can show NP-hardness of the problem of deciding whether a standard quadratic optimization problem has finitely many global minimizers. Moreover, we can show that it is NP-hard to determine whether the Lasserre hierarchy of a polynomial optimization problem has finite convergence. The key idea is to reduce it to the problem of testing critical edges, which is itself NP-hard (see Section 4.5).

**Extension to the weighted stable set problem.** Our results extend to the general setting of weighted graphs  $(G, w)$ , where  $w \in \mathbb{R}^V$  is a positive node weight vector, i.e., with  $w_i > 0$  for all  $i \in V$ . Then,  $\alpha(G, w)$  denotes the maximum weight  $w(S) = \sum_{i \in S} w_i$  of a stable set  $S$  in  $G$ , with  $\alpha(G, e) = \alpha(G)$  for the all-ones weight vector  $w = e = (1, \dots, 1)$ . The following analog of Motzkin-Straus formulation has been shown in [GHPR97]:

$$\frac{1}{\alpha(G, w)} = \min\{p_B(x) = x^T Bx : x \in \Delta_n\}, \quad (\text{M-S-weighted})$$

where the matrix  $B$  is of the form  $B = B_w + A$ , with  $(B_w)_{ii} = 1/w_i$ ,  $A_{ii} = 0$  ( $i \in V$ ),  $(B_w)_{ij} = (1/w_i + 1/w_j)/2$ ,  $A_{ij} \geq 0$  ( $\{i, j\} \in E$ ), and  $(B_w)_{ij} = A_{ij} = 0$  ( $\{i, j\} \notin E$ ). In the case  $w = e$  we have  $B_e = I + A_G$ ; hence, if we select  $A = 0$ , then we find the original Motzkin-Straus program (M-S) and if we select  $A = \varepsilon A_G$ , then we find the perturbed Motzkin-Straus formulation mentioned in the previous paragraph. There is a natural weighted analog of critical edges: call an edge  $\{i, j\}$  *w-critical* in  $G$  if there exists  $R \subseteq V$  such that both  $R \cup \{i\}$  and  $R \cup \{j\}$  are stable sets with  $\alpha(G, w) = w(R \cup \{i\}) = w(R \cup \{j\})$ . Then, program (M-S-weighted) has finitely many minimizers if and only if  $A_{ij} > 0$  for all edges  $\{i, j\} \in E$  that are *w-critical* and, in that case, the sufficient optimality conditions hold at all minimizers (see Proposition 4.13). In addition, in that case, we can show the finite convergence of the semidefinite bounds  $\vartheta^{(r)}(G, w)$  (the weighted analogs of  $\vartheta^{(r)}(G)$ ) to  $\alpha(G, w)$  when  $G$  has no *w-critical* edge (see Section 4.4).

**Exactness of low order bounds.** There is also interest in the literature in understanding when the first level of Lasserre hierarchy (also known as the Shor relaxation or the basic semidefinite relaxation) is exact when applied to quadratic optimization problems (see, e.g., the recent papers [BY20, WK21] and further references therein). For standard quadratic programs, where one wants to minimize a quadratic form  $p_M(x) = x^T Mx$  over  $\Delta_n$ , we characterize the set of matrices  $M$  for which the first level relaxation is exact. Moreover,

we show that this holds precisely when the first level relaxation is feasible (see Lemma 4.3). In the special case of problem (M-S), when  $M = I + A_G$ , the first level relaxation gives the parameter  $p_G^{(1)}$ , which will be shown to be exact (i.e., equal to  $1/\alpha(G)$ ) precisely when the graph  $G$  is a disjoint union of cliques (see Lemma 4.8).

#### 4.2. Sum-of-squares hierarchies for standard quadratic programs

Let  $M \in \mathcal{S}^n$  be a symmetric matrix and let  $p_M := x^T M x$ . We recall the following *standard quadratic optimization problem*, defined earlier in (SQP $_M$ ), asking for the minimum of  $p_M(x)$  on  $\Delta_n$ :

$$p_M^* = \min \left\{ x^T M x : x \in \Delta_n \right\}, \quad (\text{SQP}_M)$$

which can be equivalently reformulated as the problem of minimizing a quartic function over the unit sphere:

$$p_M^* = \min \left\{ (x^{\circ 2})^T M x^{\circ 2} : x \in \mathbb{R}^n, \sum_{i=1}^n x_i^2 = 1 \right\}. \quad (\text{SQP-Q})$$

We can define the corresponding sum-of-squares hierarchies for both problems (SQP $_M$ ) and (SQP-Q), and the preordering-based hierarchy for the simplex formulation (SQP $_M$ ), leading to the parameters

$$p_M^{(r)} = \max \left\{ \lambda : x^T M x - \lambda \in \mathcal{M}(\mathbf{x})_{2r} + I_{\Delta_n} \right\}, \quad (4.5)$$

$$p_{M,\mathcal{T}}^{(r)} = \max \left\{ \lambda : x^T M x - \lambda \in \mathcal{T}(\mathbf{x})_{2r} + I_{\Delta_n} \right\}, \quad (4.6)$$

$$p_{M,\mathcal{S}}^{(r)} = \max \left\{ \lambda : (x^{\circ 2})^T M x^{\circ 2} - \lambda \in \Sigma_{2r} + I_{\mathbb{S}^{n-1}} \right\}. \quad (4.7)$$

For  $r \geq 1$ , using that  $x^T J x = (\sum_{i=1}^n x_i)^2$  and that  $\sum_{i=1}^n x_i \equiv 1 \pmod{I_{\Delta_n}}$ , we can rewrite the programs (4.5) and (4.6) as

$$p_M^{(r)} = \max \left\{ \lambda : M - \lambda J \in \text{LAS}_{\Delta_n}^{(2r)} \right\}, \quad (4.8)$$

$$p_{M,\mathcal{T}}^{(r)} = \max \left\{ \lambda : M - \lambda J \in \text{LAS}_{\Delta_n, \mathcal{T}}^{(2r)} \right\}. \quad (4.9)$$

Similarly, for  $r \geq 2$  we can write the program (4.7) as

$$p_{M,\mathcal{S}}^{(r)} = \max \left\{ \lambda : M - \lambda J \in \text{LAS}_{\mathbb{S}^{n-1}}^{(2r)} \right\}. \quad (4.10)$$

Alternatively, following [BDdKRQT00, dKP02], problem (SQP $_M$ ) can be reformulated as a copositive program:

$$p_M^* = \max \left\{ \lambda : M - \lambda J \in \text{COP}_n \right\}. \quad (4.11)$$

By replacing the cone  $\text{COP}_n$  by its subcone  $\mathcal{K}_n^{(r)}$ , we now obtain the following lower bound for  $p_M^*$ :

$$\Theta_M^{(r)} := \max \left\{ \lambda : M - \lambda J \in \mathcal{K}_n^{(r)} \right\} \quad (4.12)$$

for any integer  $r \geq 0$ . Then, by Theorem 2.10, we have the following link between these hierarchies.

**Theorem 4.1.** *For any  $M \in \mathcal{S}^n$  and  $r \geq 1$ , we have:*

$$p_M^* \geq p_{M,S}^{(2r)} = \Theta_M^{(2r-2)} = p_{M,T}^{(r)} \geq p_M^{(r)}. \quad (4.13)$$

This theorem shows that, in essence, there are two different sum-of-squares bounds for standard quadratic programs. In order to analyze the finite convergence of the hierarchy  $p_M^{(r)}$ , observe that the following equivalence holds:

$$p_M^{(r)} \text{ has finite convergence to } p_M^* \iff M - p_M^* J \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}, \quad (4.14)$$

which follows from relation (4.8). Observe also that the matrix  $M - p_M^* J$  lies in the boundary  $\partial \text{COP}_n$ . Then, for showing membership in  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ , we can use Theorem 2.25. This result can only be applied when the problem

$$\min \left\{ x^\top (M - p_M^* J) x : x \in \Delta_n \right\}$$

has finitely many minimizers. This corresponds to the case when problem  $(\text{SQP}_M)$  has finitely many minimizers. Then, we have the following result that follows directly from Theorem 2.25.

**Corollary 4.2.** *Let  $M \in \mathcal{S}^n$ . Consider the problem  $(\text{SQP}_M)$  and its corresponding Lasserre hierarchy  $p_M^{(r)}$ . Assume that  $(\text{SQP}_M)$  has finitely many minimizers. If, for every minimizer  $x \in \Delta_n$  of problem  $(\text{SQP}_M)$ , it holds that*

$$(Mx)_i > p_M^* \text{ for all } i \in [n] \setminus \text{Supp}(x),$$

then  $p_M^{(r)}$  has finite convergence to  $p_M^*$ .

**4.2.1. The bound  $p_M^{(1)}$ .** Now, we characterize the set of matrices  $M$  for which the program (4.5) is feasible at order  $r = 1$ . Moreover, we prove that in that case, the program is exact, i.e.,  $p_M^{(1)} = p_M^*$ .

**Lemma 4.3.** *Given a symmetric matrix  $M \in \mathcal{S}^n$ , the following assertions are equivalent.*

- (i): *The program (4.5) is feasible for  $r = 1$ , i.e.,  $p_M^{(1)}$  is finite.*
- (ii): *There exist  $\lambda \in \mathbb{R}$  and  $a \in \mathbb{R}_+^n$  such that*

$$M - \lambda J - (ae^\top + ea^\top)/2 \succeq 0.$$

- (iii):  *$p_M^{(1)} = p_M^*$ .*

PROOF. We first prove (i)  $\iff$  (ii). Assume program (4.5) is feasible, i.e., there exist  $\lambda \in \mathbb{R}$ ,  $a \in \mathbb{R}_+^n$ ,  $Q \succeq 0$  and  $u(x) \in \mathbb{R}[x]$  such that

$$x^\top Mx - \lambda = x^\top Qx + a^\top x + (e^\top x - 1)u(x).$$

Then, there exists  $v(x) \in \mathbb{R}[x]$  such that

$$x^\top Mx - \lambda(e^\top x)^2 = x^\top Qx + (a^\top x)(e^\top x) + (e^\top x - 1)v(x).$$

Indeed, we can select  $v(x) = u(x) - \lambda(1 + e^\top x)$ , which follows from

$$\begin{aligned} x^\top Mx - \lambda(e^\top x)^2 &= x^\top Mx - \lambda + \lambda(1 - (e^\top x)^2) \\ &= x^\top Qx + a^\top x + (e^\top x - 1)(u(x) - \lambda(1 + e^\top x)). \end{aligned}$$

Hence, the quadratic polynomial  $x^\top(M - \lambda J - Q - (ae^\top + ea^\top)/2)x$  vanishes on  $\{x : e^\top x = 1\}$  and thus on  $\mathbb{R}^n$ . This implies  $M - \lambda J - Q - (ae^\top + ea^\top)/2 = 0$ , and thus (ii) holds. The argument can be clearly reversed, which shows the equivalence of (i) and (ii).

As (iii) implies (i), it suffices now to show (ii)  $\implies$  (iii). By the above argument, if (ii) holds, then we have

$$p_M^{(1)} = \sup\{\lambda : \lambda \in \mathbb{R}, a \in \mathbb{R}_+^n, M - \lambda J - (ae^\top + ea^\top)/2 \succeq 0\}. \quad (4.15)$$

Define the matrices  $A_i = (e_i e_i^\top + e e_i^\top)/2$  for  $i \in [n]$ . Then, the dual program of (4.15) reads

$$\inf\{\langle M, X \rangle : \langle J, X \rangle = 1, \langle A_i, X \rangle \geq 0 \ (i \in [n]), X \succeq 0\}. \quad (4.16)$$

As program (4.16) is strictly feasible and bounded from below by  $p_M^{(1)}$ , strong duality holds and the optimum value of (4.16) is equal to  $p_M^{(1)}$ . We now show that  $p_M^* \leq p_M^{(1)}$ . For this, let  $X$  be feasible for (4.16) and define the vector  $x = Xe$ . Then,  $x \in \Delta_n$ , since  $x_i = \langle A_i, X \rangle \geq 0$  for all  $i \in [n]$ , and  $e^\top x = \langle J, X \rangle = 1$ , which implies  $x^\top Mx \geq p_M^*$ . In addition, we have  $X - xx^\top \succeq 0$ , which follows from the fact that

$$\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0,$$

(as  $X \succeq 0$ ,  $x = Xe$  and  $e^\top Xe = 1$ ). We now show  $\langle M, X \rangle \geq x^\top Mx$ . For this, consider also a feasible solution  $(\lambda, a)$  to (4.15), then  $M - \lambda J - \sum_{i=1}^n a_i A_i \succeq 0$ . Then we have  $\langle M - \lambda J - \sum_i a_i A_i, X - xx^\top \rangle \geq 0$ , which, combined with  $\langle J, X - xx^\top \rangle = 0$  and  $\langle A_i, X - xx^\top \rangle = 0$  for all  $i \in [n]$ , implies that  $\langle M, X \rangle \geq x^\top Mx \geq p_M^*$  and thus  $p_M^{(1)} \geq p_M^*$ , as desired.  $\square$

Here is an immediate consequence of the reformulation of the parameter  $p_M^{(1)}$  given in (4.15), that we will need later.

**Lemma 4.4.** *Assume that the program (4.15) defining  $p_M^{(1)}$  is feasible, i.e.,  $M = \lambda J + Q + (ae^\top + ea^\top)/2$  for some  $\lambda \in \mathbb{R}$ ,  $Q \succeq 0$  and  $a \in \mathbb{R}_+^n$ . Then,*

for any  $i \neq j \in [n]$ , we have  $M_{ii} + M_{jj} - 2M_{ij} = Q_{ii} + Q_{jj} - 2Q_{ij} \geq 0$ . In addition, if  $M_{ii} + M_{jj} - 2M_{ij} = 0$  then  $Q(e_i - e_j) = 0$ .

PROOF. Direct verification.  $\square$

On the other hand, note that the program (4.12) defining  $\Theta_M^{(0)}$  is always feasible. Indeed,  $\lambda = \min_{i,j} M_{ij}$  provides a feasible solution, since then  $M - \lambda J$  is nonnegative and thus belongs to  $\mathcal{K}_n^{(0)}$ .

**Remark 4.5.** In view of the formulation (4.15) for the parameter  $p_M^{(1)}$ , the difference with the parameter  $p_{M,\mathcal{T}}^{(1)} = p_{M,\mathcal{S}}^{(2)} = \Theta_M^{(0)}$  lies in the fact that, while for  $p_M^{(1)}$  we search for a decomposition  $M = \lambda J + Q + (ea^T + ae^T)/2 \succeq 0$  with  $Q \succeq 0$  and  $a \in \mathbb{R}_+^n$ , in the definition of  $\Theta_M^{(0)}$  we search for a decomposition  $M = \lambda J + Q + N \succeq 0$  with  $Q \succeq 0$ , but now  $N$  can be an arbitrary entry-wise nonnegative matrix.

**4.2.2. Application to the stable set problem.** Here, we apply the above results to the formulation of the stability number  $\alpha(G)$  via the Motzkin-Straus formulation (M-S), the special instance of a standard quadratic program, where we select the matrix  $M = I + A_G$  as the extended adjacency matrix of  $G$ . We set

$$p_G := p_{A_G+I}, \quad (4.17)$$

$$p_G^{(r)} := p_{A_G+I}^{(r)}. \quad (4.18)$$

We can link the parameters  $\vartheta^{(r)}(G)$  and  $\Theta_M^{(r)}$  for the matrix  $M = I + A_G$ .

**Lemma 4.6.** For any graph  $G$  and  $r \geq 0$ , we have:  $\Theta_{I+A_G}^{(r)} = \frac{1}{\vartheta^{(r)}(G)}$ .

PROOF. Directly from the definitions of  $\vartheta^{(r)}(G)$  in (3.13) and of  $\Theta_{I+A_G}^{(r)}$  in (4.12).  $\square$

We obtain the following result as a direct application of relation (4.13).

**Corollary 4.7.** For any graph  $G$  and  $r \geq 0$ , we have

$$\frac{1}{\alpha(G)} \geq \frac{1}{\vartheta^{(2r)}(G)} \geq p_G^{(r+1)}.$$

We now use the result of Lemma 4.3 to characterize when the parameter  $p_G^{(1)}$  is feasible (and thus exact).

**Lemma 4.8.** For any graph  $G$ , the parameter  $p_G^{(1)}$  is finite or, equivalently,  $p_G^{(1)} = 1/\alpha(G)$ , if and only if  $G$  is a disjoint union of cliques.

PROOF. We use Lemma 4.3 applied to the matrix  $M = I + A_G$ . First, assume  $M = \lambda J + Q + (ae^T + ea^T)/2$  for some  $\lambda \in \mathbb{R}$ ,  $Q \succeq 0$  and  $a \in$

$\mathbb{R}_+^n$ , we show that  $G$  is a disjoint union of cliques. For this it suffices to show that  $\{1, 2\}, \{1, 3\} \in E$  implies  $\{2, 3\} \in E$ . This follows easily using Lemma 4.4. Indeed, if  $\{1, 2\} \in E$  then we have  $M_{11} + M_{22} - 2M_{12} = 0$  and thus  $Q(e_1 - e_2) = 0$ . In the same way,  $\{1, 3\} \in E$  implies  $Q(e_1 - e_3) = 0$ . This implies  $Q(e_2 - e_3) = 0$ , and thus  $M_{22} + M_{33} - 2M_{23} = 0$ , i.e.,  $\{2, 3\} \in E$ .

Conversely, assume  $G$  is a disjoint union of cliques, say  $V = C_1 \cup \dots \cup C_k$  where  $k = \alpha(G)$  and each  $C_i$  is a clique of  $G$ . We show that  $p_M^{(1)} = \frac{1}{\alpha(G)}$ . For this note that, for any  $x \in \Delta_n$ , we have

$$x^T(I + A_G)x = \sum_{i=1}^k \left( \sum_{j \in C_i} x_j \right)^2 \geq \frac{1}{k} = \frac{1}{\alpha(G)}.$$

Here, we use Cauchy-Schwartz inequality combined with  $\sum_{i=1}^k (\sum_{j \in C_i} x_j) = 1$  to derive the inner inequality. This shows  $p_M^{(1)} \geq p^*$  and thus equality holds.  $\square$

In Section 4.4, we will investigate the finite convergence of the simplex-based Lasserre hierarchy  $p_G^{(r)}$ , which, in view of Corollary 4.7, directly implies finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ . We will use Corollary 4.2. This requires to understand the structure of the global minimizers of problem (M-S), which is what we do in the next section, in the general setting of the weighted stable set problem.

### 4.3. Minimizers of the (weighted) Motzkin-Straus formulation

In this section, we prove some properties of the minimizers of the Motzkin-Straus formulation, in the general setting of the weighted stable set problem. We consider a graph  $G = ([n], E)$  equipped with positive node weights  $w \in \mathbb{R}^V$ , i.e., with  $w_i > 0$  for  $i \in V$ . A stable set  $S \subseteq V$  is said to be  $w$ -maximum if it maximizes the function  $w(S) = \sum_{i \in S} w_i$  over all stable sets of  $G$  and  $\alpha(G, w)$  denotes the maximum weight of a stable set in  $G$ . We say that an edge  $\{i, j\} \in E$  is  $w$ -critical in  $G$  if there exists a set  $R \subseteq V$  such that both sets  $R \cup \{i\}$  and  $R \cup \{j\}$  are  $w$ -maximum stable sets; note this implies  $\alpha(G, w) = w(R) + w_i = w(R) + w_j$  and thus equality  $w_i = w_j$ . When  $w = e = (1, \dots, 1)$  is the all-ones weight vector, the  $w$ -maximum stable sets are the maximum stable sets,  $\alpha(G, e) = \alpha(G)$ , and the  $w$ -critical edges are the critical edges of  $G$ .

Following [GHPR97], let us define the matrix  $B_w \in S^n$ , with entries

$$\begin{aligned} (B_w)_{ii} &= \frac{1}{w_i} \quad (i \in [n]), & (B_w)_{ij} &= \frac{1}{2} \left( \frac{1}{w_i} + \frac{1}{w_j} \right) \quad (\{i, j\} \in E), \\ & & (B_w)_{ij} &= 0 \quad (\{i, j\} \in \overline{E}), \end{aligned} \tag{4.19}$$



and the matrix spaces

$$\begin{aligned} \mathcal{N}(G) = \{A \in \mathcal{S}^n : A_{ii} = 0 \ (i \in [n]), A_{ij} \geq 0 \ (\{i, j\} \in E), \\ A_{ij} = 0 \ (\{i, j\} \in \overline{E})\}, \end{aligned} \quad (4.20)$$

$$\mathcal{M}(G, w) = B_w + \mathcal{N}(G) = \{B_w + A : A \in \mathcal{N}(G)\}, \quad (4.21)$$

so that

$$\begin{aligned} \mathcal{M}(G, w) = \{B \in \mathcal{S}^n : B_{ii} = \frac{1}{w_i} \ (i \in V), B_{ij} \geq \frac{1}{2}(B_{ii} + B_{jj}) \ (\{i, j\} \in E), \\ B_{ij} = 0 \ (\{i, j\} \in \overline{E})\}. \end{aligned} \quad (4.22)$$

For the all-ones node weights  $w = e = (1, 1, \dots, 1)$ , we have  $B_w = I + A_G$ . We will also need the set

$$\mathcal{M}^*(G, w) = \{B \in \mathcal{M}(G, w) : 2B_{ij} > B_{ii} + B_{jj} \text{ for all } \{i, j\} \text{ } w\text{-critical}\}. \quad (4.23)$$

Clearly  $\mathcal{M}^*(G, w)$  contains all matrices lying in the relative interior of  $\mathcal{M}(G, w)$  and  $\mathcal{M}^*(G, w) = \mathcal{M}(G, w)$  if there is no  $w$ -critical edge in  $G$ .

In [GHPR97] it is shown that, for any matrix  $B \in \mathcal{M}(G, w)$ , the weighted stable set problem can be reformulated via the following weighted analog of the Motzkin-Straus formulation

$$\frac{1}{\alpha(G, w)} = \min\{x^T B x : x \in \Delta_n\}. \quad (\text{M-S-weighted})$$

We now investigate the minimizers of problem (M-S-weighted), whose structure depends on the weighted graph  $(G, w)$  and on the choice of the matrix  $B$  in the set  $\mathcal{M}(G, w)$ . In particular, we will show that their number is finite precisely when  $B$  belongs to the set  $\mathcal{M}^*(G, w)$ . As mentioned earlier the property of having finitely many minimizers is indeed important in the analysis of the finite convergence of the corresponding Lasserre hierarchy.

We start with a useful property of local minimizers for a class of standard quadratic programs. The proof is essentially along the lines of the proof of [GHPR97, Theorem 5] (and is the key argument for showing the equality in (M-S-weighted)).

**Lemma 4.9.** *Consider the standard quadratic program*

$$p_M^* = \min\{p_M(x) = x^T M x : x \in \Delta_n\}, \quad (4.24)$$

where  $M$  is a matrix of the form

$$M = \begin{pmatrix} a_1 & b & c_1^T \\ b & a_2 & c_2^T \\ c_1 & c_2 & M_0 \end{pmatrix}, \quad (4.25)$$

with  $a_1, a_2 > 0$ ,  $b \in \mathbb{R}$  satisfying  $2b \geq a_1 + a_2$ ,  $c_1, c_2 \in \mathbb{R}^{n-2}$  and  $M_0 \in \mathcal{S}^{n-2}$ . Assume  $x$  is a local minimizer of problem (4.24) with  $x_1, x_2 > 0$  and define the

vectors  $\tilde{x} = x + x_2(e_1 - e_2)$  and  $\bar{x} = x - x_1(e_1 - e_2) \in \Delta_n$ . Then,  $2b = a_1 + a_2$  holds and, for any scalar  $\lambda \in [0, 1]$ , we have  $p_M(\lambda\tilde{x} + (1 - \lambda)\bar{x}) = p_M(x)$ .

PROOF. Consider the problem

$$\min_{t \in [-x_2, x_1]} p_M(x_1 - t, x_2 + t, x_3, \dots, x_n),$$

which can be rewritten as

$$\min_{t \in [-x_2, x_1]} t^2(a_1 + a_2 - 2b) + \beta t + \gamma, \quad (4.26)$$

where  $\beta, \gamma$  are scalars depending on  $M$ . By assumption,  $t = 0$  lies in the interior of the interval  $[-x_2, x_1]$  and it is a local minimizer of problem (4.26). If  $a_1 + a_2 - 2b < 0$ , then the objective function of (4.26) is strictly concave, and thus it cannot have a local minimum at an interior point of  $[-x_2, x_1]$ . Hence  $a_1 + a_2 = 2b$  holds. If  $\beta \neq 0$ , then the objective function is linear and thus it again cannot have a local minimum in the interior of  $[-x_2, x_1]$ . Hence we must have  $\beta = 0$ , so that  $p_M(x) = p_M(x_1 - t, x_2 + t, x_3, \dots, x_n)$  for any  $t \in [-x_2, x_1]$  or, equivalently,  $p_M(\lambda\tilde{x} + (1 - \lambda)\bar{x}) = p_M(x)$  for any  $\lambda \in [0, 1]$ .  $\square$

We recall a result of [GHPR97] that characterizes the global minimizers of (M-S-weighted) whose support is a stable set.

**Lemma 4.10** ([GHPR97]). *Assume  $B \in \mathcal{M}(G, w)$ . Let  $x \in \Delta_n$  and assume its support  $S = \text{Supp}(x)$  is a stable set of  $G$ . If  $x$  is a global minimizer of problem (M-S-weighted), then  $S$  is a  $w$ -maximum stable set,  $x_i = \frac{w_i}{\alpha(w, G)}$  for  $i \in S$  and  $x_i = 0$  for  $i \in V \setminus S$ .*

PROOF. The argument is classical and based on Cauchy-Schwartz inequality. We have

$$1 = \sum_{i \in S} \frac{x_i}{\sqrt{w_i}} \sqrt{w_i} \leq \sqrt{\sum_{i \in S} \frac{x_i^2}{w_i}} \sqrt{\sum_{i \in S} w_i} = \sqrt{x^T B x} \sqrt{w(S)} \leq \sqrt{x^T B x} \sqrt{\alpha(G, w)},$$

where the last two (in)equalities hold since  $S$  is a stable set. By assumption,  $x^T B x = 1/\alpha(G, w)$  since  $x$  is a global minimizer of ((M-S-weighted)). Hence, equality holds throughout. Then, equality in the first (Cauchy-Schwartz) inequality implies the desired result.  $\square$

We now characterize the global minimizers of problem (M-S-weighted).

**Proposition 4.11.** *Assume  $B \in \mathcal{M}(G, w)$ . Let  $x \in \Delta_n$  with support  $S = \text{Supp}(x)$  and let  $C_1, \dots, C_k$  denote the connected components of the graph  $G[S]$ . Then,  $x$  is a global minimizer of problem (M-S-weighted) if and only if the following conditions hold:*

- (i):  $w_i = w_j$  for all  $i, j \in C_h$  and  $h \in [k]$ ,
- (ii):  $C_h$  is a clique of  $G$  for all  $h \in [k]$ ,

- (iii):  $\sum_{i \in C_h} x_i = \frac{w_{i_h}}{\alpha(G, w)}$ , where  $i_h$  is any given node in  $C_h$ , for all  $h \in [k]$ ,  
 (iv):  $2B_{ij} = B_{ii} + B_{jj} = \frac{1}{w_i} + \frac{1}{w_j}$  for all edges  $\{i, j\}$  of  $G[S]$ .

In that case all the edges of  $G[S]$  are  $w$ -critical.

PROOF. We first show the ‘if part’. Assume that (i)-(iv) hold, we show that  $x^T Bx = 1/\alpha(G, w)$  holds. Using (i)-(iv), we obtain

$$\begin{aligned} \frac{1}{\alpha(G, w)} &\leq x^T Bx = \sum_{h=1}^k \frac{1}{w_{i_h}} \left( \sum_{i \in C_h} x_i \right)^2 \\ &= \sum_{h=1}^k \frac{1}{w_{i_h}} \left( \frac{w_{i_h}}{\alpha(G, w)} \right)^2 \\ &= \frac{1}{\alpha(G, w)^2} \sum_{h=1}^k w_{i_h}. \end{aligned}$$

Note that  $\sum_{h=1}^k w_{i_h} \leq \alpha(G, w)$  since the set  $\{i_h : h \in [k]\}$  is a stable set in  $G$ . Hence, equality holds throughout, which shows the desired result.

We now show the ‘only if’ part. Assume  $x$  is a global minimizer, we show that (i)-(iv) hold. Condition (iv) follows directly using Lemma 4.9 applied to the matrix  $B$ . Consider nodes  $i_1 \in C_1, \dots, i_k \in C_k$  lying in the different connected components of  $G[S]$ . Then,  $I = \{i_1, \dots, i_k\}$  is a stable set of  $G$ . Define the vector  $y \in \Delta_n$ , with entries  $y_{i_h} = \sum_{i \in C_h} x_i$  for  $h \in [k]$  and  $y_i = 0$  for all remaining vertices  $i \in V \setminus I$ . By applying iteratively Lemma 4.9 (with the matrix  $B$ , using the edges in a spanning tree in each connected component  $C_h$ ), we obtain that  $y^T B y = x^T B x$ . Hence,  $y$  is a global minimizer of (M-S-weighted) whose support is a stable set, and thus, by Lemma 4.10, we obtain that  $I$  is a  $w$ -maximum stable set and  $\sum_{i \in C_h} x_i = y_{i_h} = w_{i_h}/w(I)$  for all  $h \in [k]$ , so that (iii) holds. Next, we check (ii), i.e., that each component (say)  $C_1$  is a clique. Indeed, if  $i \neq j \in C_1$  are not adjacent, then the set  $\{i, j\} \cup \{i_2, \dots, i_k\}$  is stable and  $w(\{i, j\} \cup \{i_2, \dots, i_k\}) > w(\{i, i_2, \dots, i_k\}) = \alpha(G, w)$ . Moreover, the edge  $\{i, j\}$  is  $w$ -critical since both sets  $\{i, i_2, \dots, i_k\}$  and  $\{j, i_2, \dots, i_k\}$  are  $w$ -maximum stable sets. Thus (i) holds and the proof is complete.  $\square$

As a direct application, we obtain the characterization of the global minimizers of the (unweighted) Motzkin-Straus problem (M-S).

**Corollary 4.12.** *Let  $x \in \Delta_n$  with support  $S = \text{Supp}(x)$  and let  $C_1, \dots, C_k$  denote the connected components of the graph  $G[S]$ . Then,  $x$  is a global minimizer of problem (M-S) if and only if the following conditions hold:*

- (i):  $k = \alpha(G)$ ,  
 (ii):  $C_h$  is a clique for all  $h \in [k]$ ,  
 (iii):  $\sum_{i \in C_h} x_i = 1/k$  for all  $h \in [k]$ .

In that case, all the edges of  $G[S]$  are critical.

As another application, we can characterize when problem (M-S-weighted) has finitely many minimizers, and in addition, we show that in this case the sufficient optimality conditions hold at all minimizers.

**Proposition 4.13.** *Assume  $B \in \mathcal{M}(G, w)$ . The following assertions are equivalent.*

- (i): *Problem (M-S-weighted) has finitely many global minimizers.*
- (ii):  *$B_{ij} > \frac{1}{2}(\frac{1}{w_i} + \frac{1}{w_j})$  for all edges  $\{i, j\} \in E$  that are  $w$ -critical.*

In that case the global minimizers are the vectors  $x \in \Delta_n$  with entries  $x_i = w_i/\alpha(G, w)$  for  $i \in S$  and  $x_i = 0$  for  $i \in V \setminus S$ , where  $S$  is a  $w$ -maximum stable set of  $G$ . Additionally, for any minimizer  $x$  it holds that

$$(Bx)_i > \frac{1}{\alpha(G, w)}$$

for any  $i \in [n] \setminus \text{Supp}(x)$ .

PROOF. We first show (i)  $\implies$  (ii). For this, assume for contradiction that there exists a  $w$ -critical edge (say)  $\{1, 2\} \in E$  such that  $B_{12} = \frac{1}{2}(1/w_1 + 1/w_2)$ , we show that the number of minimizers is infinite. As  $\{1, 2\}$  is  $w$ -critical, there exists  $R \subseteq V$  such that both sets  $R \cup \{1\}$  and  $R \cup \{2\}$  are  $w$ -maximum stable sets. For any scalar  $t \in [0, 1]$ , consider the point  $x \in \Delta_n$  with support  $S = R \cup \{1, 2\}$  and entries  $x_1 = tw_1/\alpha(G, w)$ ,  $x_2 = (1-t)w_2/\alpha(G, w)$  and  $x_i = w_i/\alpha(G, w)$  for  $i \in R$ . Then, by Proposition 4.11,  $x$  is a minimizer for all  $t \in [0, 1]$ . Now, we show (ii)  $\implies$  (i). By Proposition 4.11  $x$  should be supported in a stable set and for any  $i \in \text{Supp}(x)$  we have  $x_i = \frac{w_i}{\alpha(G, w)}$ , showing additionally the next part of this Proposition. We are left with computing  $(Bx)_i$  for  $i \in [n] \setminus \text{Supp}(x)$ . We have  $(Bx)_i = \frac{1}{\alpha(G, w)} \sum_{j \in \text{Supp}(x)} B_{ij}w_j$ . Note that  $w_j B_{ij} \geq \frac{w_j}{2w_i} + \frac{1}{2} > \frac{1}{2}$  for all  $j \in N_S(i)$ . Hence, we have  $(Bx)_i > \frac{1}{\alpha(G, w)}$  if  $|N_S(i)| \geq 2$ . So, assume now  $|N_S(i)| = 1$ , say  $N_S(i) = \{j\}$  so that  $\sum_{j \in \text{Supp}(x)} B_{ij}w_j = B_{ij}w_j \geq \frac{w_j}{2w_i} + \frac{1}{2}$ . As  $S$  is a  $w$ -maximum stable set and the set  $S \setminus \{j\} \cup \{i\}$  is stable, we have  $w(S \setminus \{j\} \cup \{i\}) \leq w(S)$  and thus  $w_i \leq w_j$ . If  $w_j > w_i$ , then we have  $B_{ij}w_j > 0$  as desired. So, assume now  $w_i = w_j$ , which implies that the edge  $\{i, j\}$  is  $w$ -critical. Then, by assumption (ii), we must have  $w_j B_{ij} > \frac{w_j}{2w_i} + \frac{1}{2} = 1$ , which again implies shows  $(Bx)_i > \frac{1}{\alpha(G, w)}$ , as desired.  $\square$

Hence, problem (M-S-weighted) has finitely many minimizers if and only if we choose the matrix  $B$  in the set  $\mathcal{M}^*(G, w)$  as defined in (4.23). This is the case, for example, when  $B$  lies in the relative interior of  $\mathcal{M}(G, w)$  as observed in [GHPR97]. Clearly,  $\mathcal{M}^*(G, w) = \mathcal{M}(G, w)$  if there is no  $w$ -critical edge in  $G$ . In the unweighted case, one can, for instance, select  $B = I + 2A_G \in \mathcal{M}^*(G, e)$  as the perturbation of the adjacency matrix, as already observed earlier, e.g., in [Bom97, PJ96]. Recent work, e.g., in [BRZ21, HR19], uses such perturbed

(aka regularized) formulations to approximate the maximum stable problem by applying first-order methods.

#### 4.4. Finite convergence and perturbed hierarchies

In this section, we study the finite convergence of the sum-of-squares hierarchies arising by considering problem (M-S-weighted) and its copositive reformulation.

**4.4.1. Finite convergence of the Lasserre hierarchy for the (weighted) Motzkin-Straus formulation.** In this section, we study the finite convergence of the Lasserre hierarchy for the (weighted) Motzkin-Straus formulation (M-S-weighted), that is, for the hierarchies  $p_B^{(r)}$  with  $B \in \mathcal{M}(G, w)$ . As a main result, we characterize the graphs  $G$  for which the hierarchy  $p_G^{(r)}$  (i.e.,  $p_B^{(r)}$  where  $w = e$  and  $B = I + A_G$ ) has finite convergence.

**Theorem 4.14.** *Let  $G$  be a graph without twin pairs. The hierarchy  $p_G^{(r)}$  has finite convergence if and only if  $G$  is acritical.*

We recall that deleting a node belonging to a twin pair does not affect the finite convergence of the hierarchy  $p_G^{(r)}$  (see Lemma 3.10). Combining this fact with Theorem 4.14, we obtain that  $p_G^{(r)}$  has finite convergence if and only if  $G$  is obtained by replicating nodes in an acritical graph.

In Section 4.3, we showed that, if in the (weighted) Motzkin-Straus problem (M-S-weighted) we choose the matrix  $B$  to lie in the set  $\mathcal{M}^*(G, w)$  from (4.23), then there are finitely many minimizers and all of them satisfy one extra technical condition (see Proposition 4.13). Hence, we can then apply Corollary 4.2 and conclude the finite convergence of the corresponding Lasserre hierarchy  $p_B^{(r)}$  in (4.5) and thus also of the bounds  $\Theta_B^{(r)}$  in (4.12).

**Theorem 4.15.** *Let  $(G, w)$  be a weighted graph with positive node weights  $w > 0$ . Consider problem (M-S-weighted), where the matrix  $B$  belongs to  $\mathcal{M}^*(G, w)$ . Then the following holds.*

$$(i): p_B^{(r)} = \frac{1}{\alpha(G, w)} \text{ for some } r \in \mathbb{N}.$$

$$(ii): \Theta_B^{(r)} = \frac{1}{\alpha(G, w)} \text{ for some } r \in \mathbb{N}.$$

*In particular, if  $G$  has no  $w$ -critical edge, then (i), (ii) hold for any matrix  $B \in \mathcal{M}(G, w)$  and thus for the matrix  $B_w$ .*

PROOF. By Proposition 4.13, for any minimizer  $x$  we have  $(Bx)_i > \frac{1}{\alpha(G, w)}$ . Then, by Corollary 4.2, we obtain (i). Then, (ii) follows from (i) in view of Theorem 4.1.  $\square$

Applying this result to the setting  $w = e$ , we obtain finite convergence of the hierarchy  $p_G^{(r)}$  (and thus  $\vartheta^{(r)}(G)$ ) for acritical graphs.

**Corollary 4.16.** *Assume  $G$  is a graph with no critical edges. Then, the following holds.*

- (i):  $p_G^{(r)} = \frac{1}{\alpha(G)}$  for some  $r \in \mathbb{N}$ , i.e.,  $M_G \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ .
- (ii):  $\vartheta^{(r)}(G) = \alpha(G)$  for some  $r \in \mathbb{N}$ , i.e.,  $M_G \in \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ .

PROOF. This is a direct consequence of Theorem 4.15, applied to the all-one node weights  $w = e$  and the matrix  $B = I + A_G$ , in which case we have  $p_G^{(r)} = p_B^{(r)}$  and  $\vartheta^{(r)}(G) = \frac{1}{\Theta_B^{(r)}}$ .  $\square$

**4.4.2. Finite convergence and critical edges.** The result of Corollary 4.16 shows the ‘if part’ of Theorem 4.14. In order to finish the proof of Theorem 4.14, it remains to show that if  $G$  does not have twin pairs and has critical edges, then the hierarchy  $p_G^{(r)}$  does not have finite convergence. We show a more general result that we will use later in Section 4.5.

We consider a graph  $G$  without weights, i.e.,  $w = e$ , and we fix a matrix  $B \in \mathcal{M}(G)$ . That is,  $B_{ii} = 1$  for  $i \in V$ ,  $B_{ij} \geq 1$  for  $\{i, j\} \in E$  and  $B_{ij} = 0$  for  $\{i, j\} \notin E$ . Then, we have

$$\frac{1}{\alpha(G)} = \min \left\{ x^\top Bx : x \in \Delta_n \right\}. \quad (4.27)$$

We have the following result about the finite convergence of the corresponding Lasserre hierarchy  $p_B^{(r)}$  for problem (4.27).

**Theorem 4.17.** *Let  $G$  be a graph without twin pairs and let  $B \in \mathcal{M}(G)$ . The Lasserre hierarchy  $p_B^{(r)}$  has finite convergence to  $\frac{1}{\alpha(G)}$  if and only if, for any critical edge  $\{l, m\}$  of  $G$ , we have  $B_{lm} > 1$ .*

PROOF. The ‘if’ part follows directly from Theorem 4.15. For the ‘only if’ part we proceed by contradiction as follows. Assume there is a critical edge  $\{l, m\}$  such that  $B_{lm} = 1$ . We assume, moreover, that  $p_B^{(r)}$  has finite convergence, that is, there exist  $\sigma, \sigma_i \in \Sigma$  for  $i \in V$ , and  $q \in \mathbb{R}[\mathbf{x}]$  such that

$$x^\top Bx - \frac{1}{\alpha(G)} = \sigma + \sum_{i \in V} x_i \sigma_i + q \left( \sum_{i=1}^n x_i - 1 \right). \quad (4.28)$$

Since the edge  $\{l, m\}$  is critical there exists  $S \subseteq V$  such that  $S \cup \{l\}$  and  $S \cup \{m\}$  are  $\alpha$ -stable sets in  $G$ . By Proposition 4.11, for  $t \in (0, 1)$ , the vector

$$u_t = \frac{1}{\alpha(G)} (t\chi^{S \cup \{l\}} + (1-t)\chi^{S \cup \{m\}})$$

is an optimal solution of problem (4.27), i.e.,  $u_t^\top B u_t = \frac{1}{\alpha(G)}$  and  $u_t \in \Delta_n$ . We evaluate relation (4.28) at  $x + u_t$  and we obtain

$$x^\top B x + 2x^\top B u_t = \sigma(x + u_t) + \sum_{i=1}^n (x + u_t)_i \sigma_i(x + u_t) + q(x + u_t) \left( \sum_{i=1}^n x_i \right). \quad (4.29)$$

Now, we will reach a contradiction by comparing coefficients at both sides in relation (4.29). First, since there is no constant term on the left hand side the constant term on the right hand side is equal to zero. That is,

$$\sigma(u_t) + \frac{1}{\alpha(G)} \sum_{s \in S} \sigma_s(u_t) + \frac{t}{\alpha(G)} \sigma_l(u_t) + \frac{1-t}{\alpha(G)} \sigma_m(u_t) = 0.$$

This implies that, for any  $t \in (0, 1)$ , the polynomials  $\sigma(x + u_t)$ , and  $\sigma_i(x + u_t)$  (for  $i \in S \cup \{l, m\}$ ) do not have a constant term and therefore do not have linear terms. Now, we compare the coefficient of  $x_s$ , where  $s \in S$ . In the right hand side of (4.29), it is equal to  $2 \sum_{i \in S \cup \{l, m\}} B_{si}(u_t)_i = 2B_{ss}(u_t)_s = \frac{2}{\alpha(G)}$ . On the left hand side of (4.29), the polynomials  $\sigma(x + u_t)$  and  $(x + u_t)_i \sigma_i(x + u_t)$  for  $i \in S \cup \{l, m\}$  have no linear term, and for  $i \in V \setminus (S \cup \{l, m\})$ , the polynomials  $(x + u_t)_i \sigma(x + u_t)$  are divisible by  $x_i$ . Hence, the coefficient of  $x_s$  is  $q(u_t)$ . Therefore,  $q(u_t) = \frac{2}{\alpha(G)}$ . Let  $j \in V$  be such that  $j \in N_G(l)$  and  $j \notin N_G(m)$ . Here, we use that  $l$  and  $m$  are not twin nodes (we switch  $l$  and  $m$  if necessary). We compare the coefficient of  $x_j$  at both sides of (4.29). In the left hand side, the coefficient of  $x_j$  is  $2 \sum_{i \in S \cup \{l, m\}} B_{ij}(u_t)_i = \frac{2}{\alpha(G)} B_{lj} t + \frac{2}{\alpha(G)} \sum_{i \in S} B_{ij}$ . Finally, On the right hand side, the coefficient of  $x_j$  is  $\sigma_j(u_t) + q(u_t) = \sigma_j(u_t) + \frac{2}{\alpha(G)}$ . Hence, we obtain

$$\sigma_j(u_t) = \frac{2}{\alpha(G)} B_{lj} t + \frac{2}{\alpha(G)} \sum_{i \in S} B_{ij} - \frac{2}{\alpha(G)}.$$

This is a contradiction because  $\sigma_j(u_t)$  is a sum of squares of polynomials in  $t$ , while the polynomial in the right hand has degree 1 (since  $B_{lj} \geq 1$ ).  $\square$

As a direct application, taking  $B = A_G + I$  in Theorem 4.17, we obtain the ‘only if’ part of Theorem 4.14.

**4.4.3. Copositive-based bounds for the (weighted) Motzkin-Straus formulation.** Let  $(G, w)$  be a weighted graph with positive node weights  $w > 0$ . As a direct consequence of the weighted Motzkin-Straus formulation (M-S-weighted), for any matrix  $B \in \mathcal{M}(G, w)$ , we obtain the following copositive programming formulation

$$\alpha(G, w) = \min\{t : tB - J \in \text{COP}_n\} \quad (4.30)$$

for the weighted stability number. Let us write  $B = B_w + A$ , where  $A$  lies in the set  $\mathcal{N}(G)$  from (4.20). In analogy to (3.12) and (3.13), we can define the

associated linear and semidefinite bounds

$$\zeta_A^{(r)}(G, w) = \min\{t : t(B_w + A) - J \in \mathcal{C}_n^{(r)}\}, \quad (4.31)$$

$$\vartheta_A^{(r)}(G, w) = \min\{t : t(B_w + A) - J \in \mathcal{K}_n^{(r)}\}, \quad (4.32)$$

that satisfy

$$\alpha(G, w) \leq \vartheta_A^{(r)}(G, w) \leq \zeta_A^{(r)}(G, w) \text{ for all } A \in \mathcal{N}(G).$$

For the zero matrix  $A = 0$ , we may omit the index and simply write

$$\zeta_0^{(r)}(G, w) = \zeta^{(r)}(G, w) \text{ and } \vartheta_0^{(r)}(G, w) = \zeta^{(r)}(G, w).$$

In addition, in the unweighted case when  $w = e$ , we have

$$\zeta^{(r)}(G, e) = \zeta^{(r)}(G) \text{ and } \vartheta^{(r)}(G, e) = \vartheta^{(r)}(G).$$

Note also that for any matrix  $A$  we have

$$\vartheta_A^{(r)}(G, w) = \frac{1}{\Theta_{B_w+A}^{(r)}},$$

where  $\Theta_{B_w+A}^{(r)}$  is as defined in (4.12).

From the previous section, we know that the hierarchy  $\vartheta_A^{(r)}(G, w)$  converges in finitely many steps to  $\alpha(G, w)$  when the matrix  $B_w + A$  belongs to the set  $\mathcal{M}^*(G, w)$ . Recall that  $B_w + A$  belongs to the set  $\mathcal{M}^*(G, w)$  precisely when  $A \in \mathcal{N}(G)$  and  $A_{ij} > 0$  for any  $w$ -critical edge  $\{i, j\}$ . In general, one may ask whether this holds for any choice of  $A \in \mathcal{N}(G)$ . In fact, it would suffice to show this for the case  $A = 0$ , which follows from the monotonicity properties of the bounds with respect to the choice of  $A$ , shown in the next lemma.

**Lemma 4.18.** *Let  $A_1, A_2 \in \mathcal{N}(G)$ . If  $A_1 \geq A_2$  then  $\zeta_{A_1}^{(r)}(G, w) \leq \zeta_{A_2}^{(r)}(G, w)$  and  $\vartheta_{A_1}^{(r)}(G, w) \leq \vartheta_{A_2}^{(r)}(G, w)$  for all  $r \in \mathbb{N}$ . In particular, we have  $\zeta_A^{(r)}(G, w) \leq \zeta^{(r)}(G, w)$  and  $\vartheta_A^{(r)}(G, w) \leq \vartheta^{(r)}(G, w)$  for all  $A \in \mathcal{N}(G)$ .*

PROOF. Assume  $t$  is feasible for  $\zeta_{A_2}^{(r)}(G, w)$ , i.e.,  $t(B_w + A_2) - J \in \mathcal{C}_n^{(r)}$ . Then,  $t(B_w + A_1) - J = t(B_w + A_2) - J + t(A_1 - A_2) \in \mathcal{C}_n^{(r)}$  since the matrix  $t(A_1 - A_2)$  is entrywise nonnegative and thus belongs to  $\mathcal{C}_n^{(r)}$ . Hence,  $t$  is feasible for  $\zeta_{A_1}^{(r)}(G, w)$ , which shows  $\zeta_{A_1}^{(r)}(G, w) \leq \zeta_{A_2}^{(r)}(G, w)$ . The same argument shows  $\vartheta_{A_1}^{(r)}(G, w) \leq \vartheta_{A_2}^{(r)}(G, w)$ , and the last claim follows since  $A \geq 0$  for  $A \in \mathcal{N}(G)$ .  $\square$

As we now show, the linear bounds  $\zeta_A^{(r)}(G, w)$  in fact do *not* depend on the specific choice of the matrix  $A$  in  $\mathcal{N}(G)$ .

**Theorem 4.19.** *For all  $r \in \mathbb{N}$  and  $A \in \mathcal{N}(G)$ , we have*

$$\zeta_A^{(r)}(G, w) = \zeta^{(r)}(G, w).$$



PROOF. We only need to show the inequality  $\zeta_A^{(r)}(G, w) \geq \zeta^{(r)}(G, w)$ . For this, assume the matrix  $t(B_w + A) - J$  belongs to the cone  $\mathcal{C}_n^{(r)}$ , we show that also the matrix  $tB_w - J$  belongs to  $\mathcal{C}_n^{(r)}$ , which implies the desired inequality. For short, set  $B = B_w + A$ . By assumption,  $tB - J \in \mathcal{C}_n^{(r)}$ , which means that the polynomial  $(\sum_i x_i)^r x^T (tB - J)x$  has nonnegative coefficients. Following [BdK02], for any matrix  $M$  and  $r \in \mathbb{N}$ , we have

$$\left( \sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta|=r+2}} \frac{r!}{\beta!} c_\beta x^{2\beta}, \quad \text{with } c_\beta := \beta^T M \beta - \beta^T \text{diag}(M),$$

where  $\text{diag}(M) \in \mathbb{R}^n$  is the vector  $(M_{ii})_{i=1}^n$  consisting of the diagonal entries of  $M$ . Hence, the polynomial  $(\sum_i x_i)^r x^T M x$  has nonnegative coefficients if and only if  $c_\beta \geq 0$  for all  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$ . We will now prove that, for the matrix  $M = tB - J = t(B_w + A) - J$ , the property of having  $c_\beta \geq 0$  for all  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$  is in fact independent on the choice of  $A \in \mathcal{N}(G)$ . For this, let  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$ . Using the fact that  $e^T \beta = r + 2$ , we have  $c_\beta = \beta^T (tB - J)\beta - \beta^T \text{diag}(tB - J) = t(\beta^T B \beta - \beta^T \text{diag}(B_w)) - (r + 1)(r + 2)$ . Therefore,  $c_\beta \geq 0$  for all  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$  if and only if  $t\varphi^* \geq (r + 1)(r + 2)$ , where  $\varphi^*$  is defined by

$$\varphi^* := \min\{\varphi(\beta) := \beta^T B \beta - \beta^T \text{diag}(B_w) : \beta \in \mathbb{N}^n, |\beta| = r + 2\}. \quad (4.33)$$

We now show that the optimum value of the program (4.33) is attained at some  $\beta$  whose support is a stable set of  $G$ , using a similar argument as for Lemma 4.9. Assume  $\beta^* = (\beta_1^*, \beta_2^*, \dots, \beta_n^*)$  is a minimizer of problem (4.33) with  $\beta_1^*, \beta_2^* > 0$  for some edge  $\{1, 2\} \in E$ . We show that there exists another minimizer  $\beta$  of (4.33) of the form  $\beta = (\beta_1^* + \beta_2^*, 0, \beta_3^*, \dots, \beta_n^*)$  or  $(0, \beta_1^* + \beta_2^*, \beta_3^*, \dots, \beta_n^*)$ , thus with  $\beta_1 \beta_2 = 0$ . For this, we consider problem (4.33) restricted to the vectors of the form  $(\beta_1^* - \lambda, \beta_2^* + \lambda, \beta_3^*, \dots, \beta_n^*)$  with  $\lambda \in \mathbb{Z} \cap [-\beta_2^*, \beta_1^*]$ , which reads

$$\min_{\lambda \in \mathbb{Z} \cap [-\beta_2^*, \beta_1^*]} \varphi(\beta_1^* - \lambda, \beta_2^* + \lambda, \beta_3^*, \dots, \beta_n^*). \quad (4.34)$$

Observe that the objective value of problem (4.34) takes the form

$$\varphi(\beta_1^* - \lambda, \beta_2^* + \lambda, \beta_3^*, \dots, \beta_n^*) = \lambda^2 (B_{11} + B_{22} - 2B_{12}) + c\lambda + d$$

for some scalars  $c, d$ , and thus it is concave in  $\lambda$ . Hence, the minimum value of (4.34) is attained at one of the endpoints of the interval  $\mathbb{Z} \cap [-\beta_2^*, \beta_1^*]$ , which shows the desired result. Repeating this reasoning to any other edge contained in the support of  $\beta^*$ , we obtain another minimizer  $\beta$  of (4.33) whose support is a stable set of  $G$ . This shows that the optimum value of (4.33) remains the same when selecting  $A = 0$ . Therefore, if the polynomial  $(\sum_i x_i)^r x^T (tB - J)x$  has nonnegative coefficients, then also the polynomial  $(\sum_i x_i)^r x^T (tB_w - J)x$  has nonnegative coefficients. This concludes the proof.  $\square$

In [dKP02] it is shown that strict inequality  $\alpha(G) < \zeta^{(r)}(G)$  holds for all  $r \in \mathbb{N}$  when  $G$  is not a complete graph (recall Theorem 3.4). We extend this result to the weighted case and characterize when equality  $\zeta^{(r)}(G, w) = \alpha(G, w)$  holds for some  $r \in \mathbb{N}$ .

**Lemma 4.20.** *Consider a graph  $(G, w)$  with positive node weights, ordered (say) as  $w_1 \geq w_2 \geq \dots \geq w_n > 0$ , and let  $A \in \mathcal{N}(G)$ . Then, equality  $\zeta_A^{(r)}(G, w) = \alpha(G, w)$  holds for some  $r \in \mathbb{N}$  if and only if  $\alpha(G, w) = w_1$ .*

PROOF. By Theorem 4.19, it suffices to consider  $A = 0$ . Assume

$$\zeta^{(r)}(G, w) = \alpha(G, w)$$

for some  $r \in \mathbb{N}$ . Then, the polynomial  $q(x) = (\sum_i x_i)^r x^T (\alpha(G, w)B_w - J)x^T$  has nonnegative coefficients. Let  $S$  be a  $w$ -maximum stable set and let  $u$  be the corresponding minimizer (i.e. a zero of  $q(x)$ ), with entries  $u_i = w_i/\alpha(G, w)$  for  $i \in S$  and  $u_i = 0$  otherwise. We show that the coefficient of  $x_i^{r+2}$  for  $i \in S$  in  $q(x)$  is zero. Let  $c_i$  such coefficient. Since  $q$  has nonnegative coefficients we have  $0 = q(u) \geq c_i u_i^{r+2} \geq 0$ , showing that  $c_i = 0$ . On the other hand, the coefficient of  $x_i^{r+2}$  is  $-1 + \alpha(G, w)/w_i$ . Then,  $\alpha(G, w) = w_i$ . This implies that  $S = \{i\}$  and thus  $w_i = w_1 = \alpha(G, w)$ .

Conversely, assume  $\alpha(G, w) = w_1$ ; we show  $\zeta^{(r)}(G, w) = \alpha(G, w)$ , i.e., that  $M := \alpha(G, w)B_w - J \in \mathcal{C}_n^{(r)}$ , for some  $r \in \mathbb{N}$ . Note that the set  $R = \{i \in V : w_i = w_1\}$  induces a clique in  $G$ . Then, the columns/rows of  $M$  indexed by nodes in  $R$  are all identical. Since deleting repeated rows/columns preserves membership in the cone  $\mathcal{C}^{(r)}$ , we can assume without loss of generality that  $R = \{1\}$ . Hence,  $\{1\}$  is the only  $w$ -maximum stable set and the polynomial  $p_M(x) = x^T M x$  has a unique zero in the simplex, located at the corner  $e_1$ . Note also  $M_{1j} = (w_1/w_j - 1)/2 > 0$  for all  $j \in V \setminus \{1\}$ . Hence, we may apply Theorem 1.6, and conclude that there exists an  $r \in \mathbb{N}$  for which the polynomial  $(\sum_{i=1}^n x_i)^r x^T M x$  has nonnegative coefficients, so that  $M \in \mathcal{C}_n^{(r)}$ .  $\square$

In Theorem 4.19 we saw that the linear hierarchy  $\zeta_A^{(r)}(G, w)$  does not depend on the choice of  $A \in \mathcal{N}(G)$ . For the semidefinite hierarchy  $\vartheta_A^{(r)}(G, w)$  we can prove this property only for the first level of the hierarchy.

**Lemma 4.21.** *For any  $A \in \mathcal{N}(G)$  and node weights  $w > 0$ , we have  $\vartheta_A^{(0)}(G, w) = \vartheta^{(0)}(G, w)$  and thus, in particular,  $\vartheta_A^{(0)}(G) = \vartheta^{(0)}(G)$ .*

PROOF. We need to show the inequality  $\vartheta^{(0)}(G, w) \leq \vartheta_A^{(0)}(G, w)$  (the reverse follows from Lemma 4.18). For this, let  $t$  be feasible for  $\vartheta_A^{(0)}(G, w)$ , we show that  $t$  is also feasible for  $\vartheta^{(r)}(G)$ . Set  $B = B_w + A$ . By assumption, the matrix  $tB - J$  belongs to  $\mathcal{K}_n^{(0)}$ , i.e., there exists a matrix  $P \succeq 0$  such that  $\text{diag}(P) = \text{diag}(tB - J)$  and  $P \leq tB - J$  (recall the characterization of  $\mathcal{K}_n^{(0)}$  in relation (2.2)). As  $\text{diag}(tB - J) = \text{diag}(tB_w - J)$  and both  $B$  and  $B_w$  have

zero entries at positions corresponding to non-edges, it suffices to check that, for any edge  $\{i, j\} \in E$ ,  $P_{ij} \leq (tB_w - J)_{ij}$ . This follows directly from the fact  $2P_{ij} \leq P_{ii} + P_{jj} = (tB_w - J)_{ii} + (tB_w - J)_{jj} = 2(tB_w - J)_{ij}$ , where the first inequality holds since  $P \succeq 0$ .  $\square$

**Question 4.22.** *Given a weighted graph  $(G, w)$  with positive node weights  $w > 0$ , is it true that, for any  $A \in \mathcal{N}(G)$  and any  $r \in \mathbb{N}$ , we have  $\vartheta_A^{(r)}(G, w) = \vartheta^{(r)}(G, w)$ ?*

Clearly, a positive answer to this question for the all-ones node weights  $w = e$  would imply the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ . In fact, a positive answer to the following question would also suffice.

**Question 4.23.** *Given a graph  $G$ , is it true that there exists a matrix  $A \in \mathcal{N}(G)$  such that  $I + A \in \mathcal{M}^*(G, e)$  (i.e.,  $A_{ij} > 0$  for all critical edges  $\{i, j\} \in E$ ) and  $\vartheta_A^{(r)}(G) = \vartheta^{(r)}(G)$  for all  $r \in \mathbb{N}$ ?*

We will see in Chapter 6 that the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence. However, the technique used will be different from the one developed in this chapter. It remains open whether we can show the finite convergence of the parameters  $\vartheta^{(r)}(G)$  via a positive answer to Question 4.23.

## 4.5. Complexity results

As we saw earlier, having finitely many minimizers is a property that plays an important role in the study of finite convergence of the Lasserre hierarchy for polynomial optimization. This raises the question of understanding the complexity status of the following two problems. Consider a polynomial optimization problem (P) as in (1.3).

**FINITE-MIN:** Determine whether (P) has finitely many minimizers.

**FINITE-CONV:** Determine whether the corresponding Lasserre hierarchy of (P) has finite convergence.

We will show that problems (FINITE-MIN) and (FINITE-CONV) are NP-hard, already for standard quadratic programs of the form (M-S-weighted). The complexity of several other decision problems about minimizers in polynomial optimization has been studied recently in [AZ2020a, AZ2020b]. In particular, Ahmadi and Zhang [AZ2020b] show that it is strongly NP-hard to decide whether a polynomial of degree 4 has a local minimizer over  $\mathbb{R}^n$ ; they also show that the same holds for deciding if a quadratic polynomial has a local minimizer (or a strict local minimizer) over a polyhedron. In addition, they show that unless  $P=NP$  there cannot be a polynomial-time algorithm that finds a point within Euclidean distance  $c^n$  (for any constant  $c \geq 0$ ) of a local minimizer of an  $n$ -variate quadratic polynomial over a polytope.

**4.5.1. Linear programs.** Consider first the case when (P) is a linear optimization problem:

$$p^* = \inf \left\{ c^\top x : a_i^\top x \leq b_i \text{ for } i = 1, \dots, m \right\}. \quad (\text{L-P})$$

In this case, both problems (FINITE-MIN) and (FINITE-CONV) can be solved in polynomial time.

First, since the problem is convex, if  $x$  and  $y$  are two distinct global minimizers then, for every  $0 \leq t \leq 1$ , the point  $z = tx + (1-t)y$  is also a global minimizer. Hence, the problem has finitely many minimizers if and only if it has a unique one. Therefore, the problem of deciding whether a linear program has finitely many global minimizers is equivalent to the problem of deciding whether it has a unique optimal solution, and a polynomial-time algorithm for this problem was given by Appa [App02].

Now, we observe that the first level of the Lasserre sum-of-squares hierarchy for problem (L-P) finds its optimum  $p^*$ . It is easy to note that the first level of the hierarchy  $p^{(1)}$  reads

$$p^{(1)} = \sup \left\{ \lambda : c^\top x - \lambda = \sum_{i=1}^m \lambda_i (a_i^\top x - c_i), \text{ where } \lambda_i \in \mathbb{R}_+ \text{ for } i \in [m] \right\}.$$

Note that this is precisely the dual linear program of (L-P). Hence, finite convergence always holds for linear programs.

**4.5.2. Hardness in standard quadratic programs.** We show that the problems (FINITE-MIN) and (FINITE-CONV) are NP-hard already for the class of standard quadratic programs. Our approach consists in using the results from Section 4.4, combined with the fact that deciding whether an edge is critical in a graph is an NP-hard problem. We consider the following two problems.

**CRITICAL-EDGE:** Given a graph  $G = (V, E)$  without twin pairs and an edge  $e \in E$ , is  $e$  a critical edge of  $G$ ?

**STABLE-SET:** Given a graph  $G$  and  $k \in \mathbb{N}$ , does  $\alpha(G) \geq k$  hold?

The problem STABLE-SET is well-known to be NP-Complete [Kar72]. From this, we now prove that unless  $P=NP$  there is no polynomial-time algorithm to decide whether an edge is critical.

**Theorem 4.24.** *If there is a polynomial-time algorithm that solves the problem CRITICAL-EDGE, then  $P=NP$ .*

**PROOF.** Assume there is a poly-time algorithm  $A$  for solving CRITICAL-EDGE. We show that we can find the stability number of an arbitrary graph in polynomial time. Let  $G$  be a graph. We can check whether  $G$  has twin pairs in polynomial time by checking each pair of nodes and their set of neighbors. If there is a twin pair  $(u, v)$ , then update the graph  $G \rightarrow G \setminus u$  by deleting the

node  $u$ , and we have  $\alpha(G) = \alpha(G \setminus u)$ . We repeat the procedure until  $G$  has no twin pairs. Then, we take an edge  $e \in E$  and, using the algorithm A, we check if  $e$  is critical in  $G$ . We update graph  $G \rightarrow G \setminus e$  by deleting the edge  $e$ , for which  $\alpha(G \setminus e) = \alpha(G)$  if  $e$  is not critical and  $\alpha(G \setminus e) = \alpha(G) + 1$  if  $e$  is critical. We stop if the graph has no edges. This process is going to finish since at any step we delete either a node or an edge. The algorithm will finish with a graph  $\tilde{G}$  with  $|V| - d$  nodes, where  $d$  is the number of node deletions done in the process. Then, we have  $\alpha(\tilde{G}) = |V| - d = \alpha(G) + c$ , where  $c$  is the number of times we found a critical edge at the edge deletion step. Hence, we can compute  $\alpha(G)$  in poly-time using algorithm A.  $\square$

We will now use this complexity result to settle the complexity of problems FINITE-MIN and FINITE-CONV. For this, let  $G = (V, E)$  be a graph without twin pairs and let  $e \in E$ , and consider the problem

$$\frac{1}{\alpha(G)} = \min \left\{ x^\top (A_G + I + A_{G \setminus e}) x : x \in \Delta_n \right\}. \quad (4.35)$$

Here, in the matrix defining the objective function, all edges of  $G$  get weight 2, except the selected edge  $e$  which keeps weight 1. The fact that the optimum value of (4.35) is equal to  $1/\alpha(G)$  follows since this is an instance of problem (M-S-weighted) with  $B = B_w + A$ , where  $w = e$  is the all-ones weight vector,  $B_e = I + A_G$  and  $A = A_{G \setminus e}$ . We have the following result as a direct application of Proposition 4.13 and Theorem 4.17.

**Corollary 4.25.** *Let  $G = (V, E)$  be a graph without twin pairs, and let  $e \in E$  be an edge. The following assertions are equivalent.*

- (i):  $e$  is not a critical edge of  $G$ .
- (ii): Problem (4.35) has finitely many global minimizers.
- (iii): The Lasserre hierarchy of problem (4.35) has finite convergence.

PROOF. The equivalence (i)  $\iff$  (ii) follows from Proposition 4.13, and (i)  $\iff$  (iii) follows from Theorem 4.17.  $\square$

Combining Theorem 4.24 and Corollary 4.25, we obtain the following hardness results.

**Corollary 4.26.** *The problem of deciding whether a standard quadratic program has finitely many minimizers is NP-hard.*

**Corollary 4.27.** *The problem of deciding whether the Lasserre hierarchy of a standard quadratic program has finite convergence is NP-hard.*

**4.5.3. Hardness of finding  $\alpha(G)$  for acritical graphs.** We finish by showing that finding  $\alpha(G)$  is already an NP-hard problem for the class of acritical graphs.

**Proposition 4.28.** *Computing the stability number  $\alpha(G)$  is an NP-hard problem for the class of acritical graphs.*

PROOF. We show that given an arbitrary graph  $H$ , we can construct in polynomial time an acritical graph  $G$  with  $\alpha(G) = 2\alpha(H)$ . Thus, computing  $\alpha(G)$  is NP-hard. We construct  $G$  as follows: For any vertex  $v$  of  $H$  we construct two vertices  $v_1, v_2$  in  $G$ , and for any edge  $\{v, w\}$  in  $H$ , we construct the four edges  $\{v_1, w_1\}, \{v_1, w_2\}, \{v_2, w_1\}$  and  $\{v_2, w_2\}$  in  $G$ . First, observe that if  $S_G$  is stable in  $G$ , then the set  $S_H = \{v : v_1 \in S \text{ or } v_2 \in S\}$  is stable in  $H$ . Hence,  $|S_H| \leq \alpha(H)$ . Since  $|S_G| \leq 2|S_H|$ , we obtain  $\alpha(G) \leq 2\alpha(H)$ . Now, if  $S_H$  is stable in  $H$ , then the set  $S_G = \{v_1 : v \in S_H\} \cup \{v_2 : v \in S_H\}$  is stable in  $G$ , and thus  $\alpha(G) \geq 2\alpha(H)$ . Then, we have  $\alpha(G) = 2\alpha(H)$  and, moreover, all maximum stable sets of  $G$  take the form  $S_G = \{v_1 : v \in S_H\} \cup \{v_2 : v \in S_H\}$ , where  $S_H$  is a maximum stable set in  $H$ . This implies that the symmetric difference between two different maximum stable sets of  $G$  is at least 4. Thus, in view of Observation 3.12,  $G$  is acritical.  $\square$

## Low order sum-of-squares bounds for the stability number

*This chapter is mainly based on my work [LV22b] with Monique Laurent. It also includes some new results that have not been published. In particular, all results and the discussion from Section 5.5, about constructing graphs with high  $\nu$ -rank, are new.*

In this chapter, we investigate new tools for computing (and bounding) the parameter  $\vartheta$ -rank( $G$ ) (defined in Definition 3.9) for some classes of graphs. We give special attention to the study of the graphs with  $\vartheta$ -rank 0 and 1. Another contribution of this chapter is investigating the behavior of the  $\vartheta$ -rank under the simple graph operation of adding an isolated node. This graph operation turns out to be important in the analysis of the convergence of the hierarchy  $\vartheta^{(r)}$ , as pointed out in Chapter 3 (see also [GL07]). In what follows we briefly describe the main topics of this chapter with their motivation and the main contributions.

**Membership in the cones  $\mathcal{K}_n^{(0)}$  and  $\mathcal{K}_n^{(1)}$ .** A central topic of this chapter is an analysis of the graphs with  $\vartheta$ -rank 0 or 1, i.e., the graphs for which the matrix  $M_G = \alpha(G)(A_G + I) - J$  belongs to  $\mathcal{K}_n^{(0)}$  or to  $\mathcal{K}_n^{(1)}$ . For this, we will use the explicit characterization of the cones  $\mathcal{K}_n^{(0)}$  and  $\mathcal{K}_n^{(1)}$  provided by Parrilo [Par00]. As we recalled in Chapter 2 (see also relation (5.2)),  $M \in \mathcal{S}^n$  belongs to  $\mathcal{K}_n^{(0)}$  if and only if  $M$  admits a decomposition  $M = P + N$  with  $P \succeq 0$ ,  $N \geq 0$  and  $N_{ii} = 0$  for all  $i \in [n]$ ; we call such matrix  $P$  a  $\mathcal{K}^{(0)}$ -certificate for  $M$ . Similarly, a matrix  $M$  belongs to  $\mathcal{K}_n^{(1)}$  if there exist positive semidefinite matrices  $P(1), P(2), \dots, P(n)$  satisfying some linear constraints (see Lemma 5.1); 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 the matrices in the  $\mathcal{K}^{(0)}$ - and  $\mathcal{K}^{(1)}$ -certificates for  $M$ . In some cases, this permits to show uniqueness of the certificates, a useful property for the study of the  $\vartheta$ -rank. As an example, the Horn matrix  $H$  (which is equal to the graph matrix  $M_{C_5}$  of the 5-cycle) has a unique  $\mathcal{K}^{(1)}$ -certificate and this uniqueness property permits to characterize the diagonal scalings of  $H$  that belong to  $\mathcal{K}_5^{(1)}$  (see Section 5.1).

**Graphs with  $\vartheta$ -rank 0.** The study of the graphs with  $\vartheta$ -rank 0 is relevant to the question of understanding when the basic semidefinite relaxation (also known as the Shor relaxation) of a quadratic (or, more generally, polynomial) optimization problem is exact. This question has received increased attention in the years. We refer, e.g., to the works [BY20, GY21, WK21] (and references therein), which investigate this question for various classes of quadratic problems, such as random instances in [BY20] and standard quadratic programs in [GY21].

Another motivation for the study of the graphs with  $\vartheta$ -rank 0 comes from its relevance to fundamental questions in complexity theory. Deciding whether a graph  $G$  has  $\vartheta\text{-rank}(G) = 0$  amounts to deciding whether the polynomial  $f_G(x) = (x^{\circ 2})^T M_G x^{\circ 2}$  is a sum of squares, i.e., whether an associated semidefinite program is feasible. Equivalently, as mentioned above,  $\vartheta\text{-rank}(G) = 0$  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 was shown in [PK97] 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 was shown in [Ram97] 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.

Our main results about graphs with  $\vartheta$ -rank 0 are as follows. We characterize the critical graphs with  $\vartheta$ -rank 0 as the disjoint unions of cliques, and we reduce the problem of deciding whether a graph has  $\vartheta$ -rank 0 to the same problem for the class of acritical graphs (see Section 5.3). This reduction can be done in polynomial time for the class of graphs  $G$  with a fixed value of  $\alpha(G)$ .

We recall that in Chapter 4 (Lemma 4.8), we fully characterized the graphs for which the parameter  $p_G^{(1)}$  is exact (i.e., when  $p_G^{(1)} = 1/\alpha(G)$ ) also as the disjoint union of cliques. In contrast, finding a characterization for the graphs for which  $\vartheta^{(0)}(G) = \alpha(G)$  seems much more challenging.

**Isolated nodes and graphs with  $\vartheta$ -rank 1.** In [GL07] it was conjectured that adding an isolated node to a graph does not increase the  $\vartheta$ -rank (see Conjecture 4 in [GL07]). Additionally, it was shown that a positive answer to this conjecture would imply a positive answer to Conjecture 3.7. In this chapter, we show that adding an isolated node to a graph with  $\vartheta$ -rank 1 may produce a graph with  $\vartheta$ -rank at least 2, thus disproving the conjecture from [GL07]. We also characterize the maximum number of isolated nodes that can be added to some graphs with  $\vartheta$ -rank 1 (such as odd cycles and their



complements) while preserving the  $\vartheta$ -rank 1 property (see Section 5.4). For example, for the graph  $C_5$ , this maximum number of nodes is shown to be equal to 8.

Nevertheless, studying the behaviour of the  $\vartheta$ -rank after adding an isolated node also plays a role for studying the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ . We show that we have finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  for every graph if and only if adding an isolated node preserves the finiteness of the  $\vartheta$ -rank (see Proposition 5.19). In fact, this reduction will be used later in Chapter 6 for showing the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$ .

**Parameters  $\nu^{(r)}$  and membership in the cones  $\mathcal{Q}_n^{(r)}$ .** In Section 5.5, we analyze the parameters  $\nu^{(r)}(G)$  which arises naturally by changing the cones  $\mathcal{K}_n^{(r)}$  by the cones  $\mathcal{Q}_n^{(r)}$  in the definition of the parameters  $\vartheta^{(r)}(G)$ . These parameters converge asymptotically to  $\alpha(G)$  as  $r \rightarrow \infty$ . We construct classes of graphs for which the hierarchy  $\nu^{(r)}(G)$  takes an unbounded number of steps to converge to  $\alpha(G)$ , partially solving an open question from [PVZ07] and [DV15]. For this, we extend the techniques developed in Section 5.1 for testing the membership in the cones  $\mathcal{K}_n^{(0)}$  and  $\mathcal{K}_n^{(1)}$  to study the membership in the cones  $\mathcal{Q}_n^{(r)}$ .

### 5.1. Preliminaries on the cones $\mathcal{K}_n^{(0)}$ and $\mathcal{K}_n^{(1)}$

We recall the reformulation (1.24) of the cones  $\mathcal{K}_n^{(r)}$  given by Peña, Vera and Zuluaga in [ZVP06] as an application of Theorem 1.14:

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left( \sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| \leq r+2}} \sigma_\beta x^\beta \text{ for some } \sigma_\beta \in \Sigma_{r+2-|\beta|} \right\},$$

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

$$x^T M x = x^T P x + \sum_{0 \leq i < j \leq n} c_{ij} x_i x_j. \quad (5.1)$$

This corresponds to the characterization shown in (2.2) of the cone  $\mathcal{K}_n^{(0)}$  given by Parrilo in [Par00]. We recall this relation:

$$\mathcal{K}_n^{(0)} = \{ P + N : P \succeq 0, N \geq 0 \}. \quad (5.2)$$

Note that in (5.2) we can indeed assume, without loss of generality, that  $N_{ii} = 0$  for all  $i \in [n]$ . We say that  $P$  is a  $\mathcal{K}^{(0)}$ -certificate for  $M$  if  $P \succeq 0$ ,  $P \leq M$  and  $P_{ii} = M_{ii}$  for all  $i \in [n]$ . In other words,  $P$  is a  $\mathcal{K}^{(0)}$ -certificate for  $M$  if there exist scalars  $c_{ij} \geq 0$  for  $1 \leq i < j \leq n$  for which equation (5.1) holds.

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

$$\left( \sum_{i=1}^n x_i \right) x^T M x = \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k. \quad (5.3)$$

From this, we get the characterization of the cone  $\mathcal{K}_n^{(1)}$  from Parrilo [Par00] (see also [dKP02]).

**Lemma 5.1.** *A matrix  $M$  belongs to the cone  $\mathcal{K}_n^{(1)}$  if and only if there exist matrices  $P(i) \succeq 0$  for  $i \in [n]$  and scalars  $c_{ijk} \geq 0$  for  $1 \leq i < j < k \leq n$  satisfying Equation (5.3). Equivalently, there exist matrices  $P(i) \in \mathcal{S}^n$  for  $i \in [n]$  satisfying the following conditions:*

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

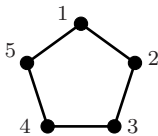
PROOF. As observed above,  $M \in \mathcal{K}_n^{(1)}$  if and only if there exist matrices  $P(i) \succeq 0$  for  $i \in [n]$  and scalars  $c_{ijk} \geq 0$  satisfying Eq.(5.3). We now obtain the conditions (ii)-(iv) by comparing coefficients at both sides of (5.3). We give the details since they will be useful later. First, we start with the left hand side in (5.3):

$$\begin{aligned} \left( \sum_{i=1}^n x_i \right) x^T M x &= \sum_{i=1}^n M_{ii} x_i^3 + \sum_{i \neq j \in [n]} x_i^2 x_j (M_{ii} + 2M_{ij}) \\ &+ \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (M_{ij} + M_{jk} + M_{ik}). \end{aligned} \quad (5.4)$$

Now, we expand the right hand side in (5.3):

$$\begin{aligned} \sum_{i=1}^n x_i x^T P(i) x + \sum_{1 \leq i < j < k \leq n} c_{ijk} x_i x_j x_k &= \sum_{i=1}^n x_i^3 P(i)_{ii} \\ &+ \sum_{i \neq j \in [n]} x_i^2 x_j (P(j)_{ii} + 2P(i)_{ij}) \\ &+ \sum_{1 \leq i < j < k \leq n} x_i x_j x_k (P(i)_{jk} + P(j)_{ik} + P(k)_{ij} + c_{ijk}). \end{aligned} \quad (5.5)$$

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

FIGURE 5.1. Graph  $C_5$ 

**Remark 5.2.** Observe that Lemma 5.1 remains valid if in (i) we replace the condition  $P(i) \succeq 0$  by the weaker condition  $P(i) \in \mathcal{K}_n^{(0)}$ . Indeed, since  $\mathcal{K}_n^{(0)} = \mathcal{S}_+^n + \mathbb{R}_+^{n \times n}$ , the ‘only if’ part is clear since  $\mathcal{S}_+^n \subseteq \mathcal{K}_n^{(0)}$ , and the ‘if part’ follows easily from the fact that  $(x^{\circ 2})^T N x^{\circ 2} \in \Sigma$  for any  $N \in \mathbb{R}_+^{n \times n}$ .

We say that the matrices  $P(1), P(2), \dots, P(n)$  are a  $\mathcal{K}^{(1)}$ -certificate for  $M$  if they satisfy the conditions (i)-(iv) of Lemma 5.1. 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 (5.3).

Now we show two results about  $\mathcal{K}^{(0)}$ - and  $\mathcal{K}^{(1)}$ -certificates, involving their kernel, that will be repeatedly used in this chapter.

**Lemma 5.3.** Let  $M \in \mathcal{K}_n^{(0)}$  and let  $P$  be a  $\mathcal{K}^{(0)}$ -certificate of  $M$ . If  $x \in \mathbb{R}_+^n$  and  $x^T M x = 0$ , then  $Px = 0$  and  $P[S] = M[S]$ , where  $S = \{i \in [n] : x_i > 0\}$  is the support of  $x$ .

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

**Lemma 5.4.** Let  $M \in \mathcal{K}_n^{(1)}$  and let  $P(1), \dots, P(n)$  be a  $\mathcal{K}^{(1)}$ -certificate of  $M$ . Let  $x \in \mathbb{R}_+^n$  such that  $x^T M x = 0$ . Then the following holds:

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

PROOF. By evaluating Equation (5.3) at  $x$ , we get that the left hand side is zero while all terms on the right hand side are nonnegative, so all of them vanish. Hence, if  $x_i > 0$  then  $x^T P(i)x = 0$ , which implies  $P(i)x = 0$  as  $P(i) \succeq 0$ . On the other hand, if  $x_i x_j x_k > 0$  then  $c_{ijk} = 0$ , which implies the desired identity (see Equation (5.4) and Equation (5.5)).  $\square$

**Example 5.5.** Consider the 5-cycle  $C_5$  shown in Figure 5.1 and its associated graph matrix  $M_{C_5} = 2(A_{C_5} + I) - J$ , equal the Horn matrix;

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

The Horn matrix  $H$  is known to belong to  $\mathcal{K}_n^{(1)}$  [Par00]. As we now show, it admits a unique  $\mathcal{K}^{(1)}$ -certificate, where the matrices  $P(1), \dots, P(5)$  are of the form shown below:

$$P(1) = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 \end{pmatrix}, \quad P(i) = \begin{pmatrix} \overbrace{1 & 1 & 1}^{i^\perp} & \overbrace{-1 & -1}^{v \setminus i^\perp} \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 \end{pmatrix} \quad \text{for } i \in [5]. \quad (5.6)$$

Here,  $i^\perp$  denote the extended neighborhood of  $i$ , i.e.,  $\{i\} \cup N_G(i)$ . Up to symmetry it suffices to show that  $P(1)$  has the above shape. Let  $C_1, C_2, C_3, C_4, C_5$  denote its columns. Since the vectors  $(1, 0, 1, 0, 0)$ ,  $(1, 0, 0, 1, 0)$ ,  $(1, 1, 0, 2, 0)$ ,  $(1, 0, 2, 0, 1)$  are zeros of the form  $x^T H x$ , by Lemma 5.4 (i), we obtain  $C_1 = -C_3$ ,  $C_1 = -C_4$ ,  $C_1 + C_2 + 2C_4 = 0$  and  $C_1 + C_5 + 2C_3 = 0$ . Hence,  $C_1 = C_2 = C_5 = -C_3 = -C_4$ . Since  $P(1)_{11} = 1$  the above conditions determine the first row and column and therefore the rest of the matrix  $P(1)$ , which thus has the desired shape.

**Characterizing the diagonal scalings of the Horn matrix in  $\mathcal{K}_5^{(1)}$ .** As shown in Chapter 2, for studying the question of whether the union  $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$  covers the full cone  $\text{COP}_5$ , it is crucial to understand the membership of the Horn matrix and its diagonal scalings in the cones  $\mathcal{K}_5^{(r)}$  (recall Theorem 2.3). Here, we give a full characterization of the diagonal scalings of the Horn matrix that belong to  $\mathcal{K}_5^{(1)}$ . A key ingredient for this is the fact that the Horn matrix admits a unique  $\mathcal{K}^{(1)}$ -certificate, as was observed in Example 5.5.

**Theorem 5.6.** *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*

$$d_{i-1}d_i + d_i d_{i+1} \geq d_{i-1}d_{i+1} \quad \text{for } i \in [5] \text{ (indices taken modulo 5)}. \quad (5.7)$$

PROOF. Set  $M := DHD$ . First, we show the ‘if part’. Assume  $d_1, \dots, d_5$  satisfy conditions (5.7); 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 (5.6); we show that the matrices  $Q(i)$  form a  $\mathcal{K}^{(1)}$ -certificate for  $M$ , i.e., satisfy the conditions (i)-(iv) from Lemma 5.1. Clearly,  $Q(i) \succeq 0$  and  $Q(i)_{ii} = d_i^2$  for all  $i \in [5]$ , so (i), (ii) hold. Also,  $2Q(i)_{ij} + Q(j)_{ii} = 2d_i d_j P(i)_{ij} + d_j^2 P(j)_{ii} = 2M_{ij} + M_{ii}$  since  $P(i)_{ij} = H_{ij}$  and  $P(j)_{ii} = H_{ii}$ , so (iii) holds. We now check

(iv), i.e.,  $Q(i)_{jk} + Q(j)_{ik} + Q(k)_{ij} \leq M_{ij} + M_{jk} + M_{ik}$  for any distinct  $i, j, k \in [5]$ . There are two possible patterns (up to symmetry):  $(i, j, k) = (1, 2, 4)$  and  $(i, j, k) = (5, 1, 2)$ . For the first pattern, we get

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

For the second pattern we get

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

which is nonnegative if and only if (5.7) holds. Hence, the conditions (5.7) indeed imply that the condition (iii) of Lemma 5.1 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 (5.6). In view of the above, this implies that the  $d_i$ 's satisfy the conditions (5.7), as desired. Up to symmetry, it suffices to show  $Q(1) = DP(1)D$ . For this note that if  $z^T H z = 0$  for  $z \in \mathbb{R}_+^n$ , then  $y^T M y = 0$  for  $y := D^{-1}z \in \mathbb{R}_+^n$  and thus, by Lemma 5.4,  $Q(i)y = 0$  whenever  $y_i > 0$ . Consider the vectors  $z_1 = (1, 0, 1, 0, 0)$ ,  $z_2 = (1, 0, 0, 1, 0)$ ,  $z_3 = (1, 1, 0, 2, 0)$ ,  $z_4 = (1, 0, 2, 0, 1)$ , which are zeros of  $x^T H x$ , and the corresponding vectors  $y_i = D^{-1}z_i$  for  $i = 1, 2, 3, 4$ , which are zeros of  $x^T M x$ . Let  $C_1, \dots, C_5$  denote the columns of  $Q(1)$ . Then, using the zeros  $y_1, \dots, y_5$  of  $x^T M x$  we obtain the relations

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

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

**Zeros of the form  $x^T M_G x$ .** 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 graph matrices  $M_G = \alpha(G)(A_G + I) - J$  we have a full characterization of the zeros of the associated quadratic form in  $\Delta_n$  (and thus in  $\mathbb{R}_+^n$ ). As observed in Chapter 4, for  $x \in \Delta_n$ , we have  $x^T M_G x = 0$  if and only if  $x$  is an optimal solution of the program (M-S):

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

Indeed, we have

$$x^T M_G x = 0 \iff \alpha(G)x^T (A_G + I)x - x^T J x = 0 \iff x^T (A_G + I)x = \frac{1}{\alpha(G)}. \quad (5.8)$$

By Proposition 4.11, we have a full characterization of the zeros of the form  $x^T M_G x$  in  $\Delta_n$ . This characterization holds in the more general setting of weighted graphs. Here, we recall the result of Proposition 4.11 for the case of unweighted graphs.

**Theorem 5.7.** *Let  $x \in \Delta_n$  with support  $S = \{i \in [n] : x_i > 0\}$ , and let  $V_1, V_2, \dots, V_k$  denote the connected components of the graph  $G[S]$ . Then,  $x$  is an optimal solution of (M-S) if and only if  $k = \alpha(G)$ ,  $V_i$  is a clique and  $\sum_{j \in V_i} x_j = \frac{1}{\alpha(G)}$  for all  $i \in [k]$ . In that case, all edges in  $G[S]$  are critical edges of  $G$ .*

In particular, if  $S$  is a stable set of size  $\alpha(G)$ , then we have

$$(\chi^S)^T M_G \chi^S = 0. \quad (5.9)$$

## 5.2. $\vartheta$ -rank, simple graph operations and some examples

Recall that the  $\vartheta$ -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  $\vartheta$ -rank based on simple graph operations. Namely, we investigate the role of isolated nodes and critical edges, and their impact on the convergence behavior of the hierarchy  $\vartheta^{(r)}(G)$ . In particular, we will show that the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence to  $\alpha(G)$  for every graph if and only if the  $\vartheta$ -rank remains finite under the operation of adding isolated nodes. This reduction will be used in Chapter 6 for showing the finite convergence of the hierarchy  $\vartheta^{(r)}$ .

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

**Lemma 5.8.** *Let  $G = (V = [n], E)$  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. Assume  $G$  and  $H$  have, respectively,  $n$  and  $m$  nodes and we assume the nodes of  $H$  are  $\{1, 2, \dots, m\}$ . 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  $M_G$ . Assume  $\vartheta\text{-rank}(G) = r$ , hence  $M_G \in \mathcal{K}_n^{(r)}$ , that is,  $(\sum_{i=1}^n x_i^2)^r (x^{\circ 2})^T M_G x^{\circ 2}$  is a sum of squares. By setting  $x_i = 0$  for  $i \in \{m+1, \dots, n\}$ , we obtain that  $(\sum_{i=1}^m x_i^2)^r (x^{\circ 2})^T M_H x^{\circ 2}$  is a sum of squares, thus  $M_H \in \mathcal{K}_m^{(r)}$ , so  $\vartheta\text{-rank}(H) \leq r$ .  $\square$

**Remark 5.9.** *Let  $G$  be the graph obtained by adding a pendant edge to  $C_5$  (see the leftmost graph in Fig. 5.2), so that  $\alpha(G) = 3 = \alpha(C_5) + 1$ . Then,  $G$  has  $\vartheta$ -rank 0 as it can be covered by  $\alpha(G) = 3$  cliques (see relation 5.14). However,  $C_5$  is an induced subgraph of  $G$  and has  $\vartheta$ -rank 1 (see Example 5.5). This shows that the condition of having the same stability number in Lemma 5.8 cannot be dropped.*

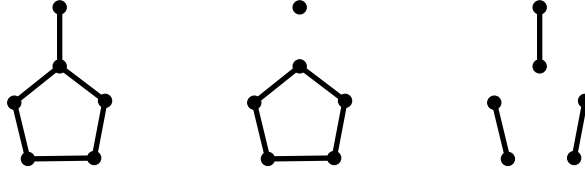


FIGURE 5.2. Graph  $G$  (left), graph  $H_1$  (middle), graph  $H_2$  (right)

**5.2.1. Role of critical edges.** In this section, we present two results that are useful for bounding the  $\vartheta$ -rank and show the role of critical edges in this context. On the one hand, deleting non-critical edges can only increase the  $\vartheta$ -rank. On the other hand, we can strengthen a result from [GL07] for the class of acritical graphs.

**Lemma 5.10.** *Let  $G = (V, E)$  be a graph and let  $e \in E$ . If  $e$  is not a critical edge, i.e.,  $\alpha(G) = \alpha(G \setminus e)$ , then  $\vartheta\text{-rank}(G) \leq \vartheta\text{-rank}(G \setminus e)$ .*

PROOF. Assume  $M_{G \setminus e} \in \mathcal{K}_n^{(r)}$ . Then,  $M_G = M_{G \setminus e} + (M_G - M_{G \setminus e})$  belongs to  $\mathcal{K}_n^{(r)}$ , since  $M_G - M_{G \setminus e} = \alpha(G)(A_G - A_{G \setminus e})$  is a nonnegative matrix and thus belongs to  $\mathcal{K}_n^{(r)}$ .  $\square$

Hence, it suffices to show Conjecture 3.7 (i.e.,  $\vartheta\text{-rank}(G) \leq \alpha(G) - 1$  for all graphs  $G$ ) and Theorem 3.8 (i.e.,  $\vartheta\text{-rank}(G) < \infty$  for all graphs  $G$ ) for the class of critical graphs.

**Remark 5.11.** *Let  $G = (V, E)$  be a graph. Then, one can find a subgraph  $H = (V, F)$  of  $G$  (with  $F \subseteq E$ ), which is critical and has the same stability number:  $\alpha(G) = \alpha(H)$ . Indeed, to get such a graph  $H$  it suffices to delete successively any non-critical edge until getting a subgraph where all edges are critical. Then, by Lemma 5.10, for any such  $H$  we have*

$$\vartheta\text{-rank}(G) \leq \vartheta\text{-rank}(H). \quad (5.10)$$

As shown in Example 5.12 below the inequality (5.10) can be strict.

**Example 5.12.** *Consider the graph  $G$  in Figure 5.2, obtained by adding one pendant node to the cycle  $C_5$ . Then,  $\alpha(G) = 3 = \bar{\chi}(G)$  and thus we have  $\vartheta\text{-rank}(G) = 0$ . Note that  $G$  has two critical subgraphs  $H_1$  and  $H_2$  with  $\alpha(H_1) = \alpha(H_2) = 3$ , shown in Figure 5.2:  $H_1$  is  $C_5$  with an isolated node, which has  $\vartheta\text{-rank}(H_1) = 1$  (see, e.g., [dKP02] or Corollary 5.56), while  $H_2$  consists of three independent edges with  $\vartheta\text{-rank}(H_2) = 0$  (since  $\alpha(H_2) = \bar{\chi}(H_2) = 3$ ).*

In the above lemma it was observed that critical edges play a role in the study of the  $\vartheta$ -rank, namely it would suffice to bound the  $\vartheta$ -rank of critical

graphs. On the other hand, we now prove a stronger version of Conjecture 3.7 for acritical graphs with  $\alpha(G) \leq 8$ . In [GL07] the authors proposed the following conjecture and proved that it implies Conjecture 3.7.

**Conjecture 5.13** ([GL07]). *For any  $r \geq 1$ , we have*

$$\vartheta^{(r)}(G) \leq r + \max_{S \subseteq V, S \text{ stable}, |S|=r} \vartheta^{(0)}(G \setminus S^\perp). \quad (5.11)$$

**Theorem 5.14** ([GL07]). *Conjecture 5.13 holds for  $r \leq \min(6, \alpha(G) - 1)$  and for  $r = 7 = \alpha(G) - 1$ . In particular, Conjecture 3.7 holds for graphs with  $\alpha(G) \leq 8$ , i.e.,  $\vartheta$ -rank( $G$ )  $\leq \alpha(G) - 1$ .*

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

**Proposition 5.15.** *Let  $G$  be an acritical graph with  $\alpha(G) \leq 8$ . Then,  $\vartheta$ -rank( $G$ )  $\leq \alpha(G) - 2$ .*

PROOF. It suffices to show  $\vartheta^{(0)}(G \setminus S^\perp) \leq 2$  if  $S$  is stable of size  $\alpha(G) - 2$  since then the result follows from relation (5.11). 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 ([CRST06]),  $G \setminus S^\perp$  contains  $C_5$  or  $\overline{C_{2n+1}}$  ( $n \geq 2$ ) as an induced subgraph. Since these graphs have stability number equal to  $\alpha(G \setminus S^\perp) = 2$  they must be acritical graphs by the above argument. Thus we reach a contradiction since  $C_5$  and  $\overline{C_{2n+1}}$  have critical edges. Hence,  $G \setminus S^\perp$  is perfect and thus we have  $\vartheta^{(0)}(G \setminus S^\perp) = \alpha(G \setminus S^\perp) = 2$ , which completes the proof.  $\square$

**5.2.2. Role of isolated nodes.** Recall that the graph  $G \oplus i$  is the graph obtained by adding the isolated node  $i$  to the graph  $G$ . We recall a result from [GL07], which is useful for bounding the  $\vartheta$ -rank of a graph in terms of the  $\vartheta$ -rank of certain subgraphs with an added isolated node. We recall also the proof of this result for the sake of completeness.

**Proposition 5.16** ([GL07]). *For any graph  $G = (V, E)$  we have:*

$$\vartheta\text{-rank}(G) \leq 1 + \max_{i \in V} \vartheta\text{-rank}((G \setminus i^\perp) \oplus i). \quad (5.12)$$

PROOF. Set  $G_i := G \setminus i^\perp \oplus K_{i^\perp}$ . By applying Lemma 3.10 repeatedly, we have  $\vartheta\text{-rank}(G_i) = \vartheta\text{-rank}(G \setminus i^\perp \oplus i)$ . Assume that  $M_{G_i} \in \mathcal{K}_n^{(r-1)}$  for all



$i \in V$ , we prove that  $M_G \in \mathcal{K}_n^{(r)}$ . Note that each matrix

$$P(i) := M_{G_i} + (\alpha(G) - \alpha(G_i))(I + A_{G_i}) = \alpha(G)(I + A_{G_i}) - J$$

belongs to  $\mathcal{K}_n^{(r-1)}$ , since it is the sum of two matrices in  $\mathcal{K}_n^{(r-1)}$  as  $\alpha(G) - \alpha(G_i) \geq 0$ . We have

$$\begin{aligned} & \left( \sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^T M_G x^{\circ 2} \\ &= \left( \sum_{i=1}^n x_i^2 \right)^{r-1} \left( \sum_{i=1}^n x_i^2 (x^{\circ 2})^T P(i) x^{\circ 2} + \sum_{i=1}^n x_i^2 (x^{\circ 2})^T (M_G - P(i)) x^{\circ 2} \right) \\ &= \sum_{i=1}^n x_i^2 \underbrace{\left( \sum_{i=1}^n x_i^2 \right)^{r-1} (x^{\circ 2})^T P(i) x^{\circ 2}}_{=\sigma_1} \\ & \quad + \underbrace{\left( \sum_{i=1}^n x_i^2 \right)^{r-1} \left( \sum_{i=1}^n x_i^2 (x^{\circ 2})^T (M_G - P(i)) x^{\circ 2} \right)}_{=\sigma_2}. \end{aligned}$$

We show that this polynomial is a sum of squares, thus showing  $M_G \in \mathcal{K}_n^{(r)}$ . Indeed,  $\sigma_1 \in \Sigma$  since each  $P(i)$  belongs to  $\mathcal{K}_n^{(r-1)}$ . In addition, one can check that the matrices  $P(i)$  satisfy the conditions (ii)-(iv) of Lemma 5.1. Then, using the identity (5.3) we obtain that  $\sigma_2$  has nonnegative coefficients, and thus  $\sigma_2 \in \Sigma$ , which concludes the proof.  $\square$

In view of Proposition 5.16, understanding how adding isolated nodes changes the  $\vartheta$ -rank is crucial for understanding the convergence behavior of the bounds  $\vartheta^{(r)}(G)$ . On the one hand, it was shown in [GL07] that if adding an isolated node does not increase the  $\vartheta$ -rank, then Conjecture 3.7 holds.

**Proposition 5.17** ([GL07]). *Assume  $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G)$  for any graph  $G$ . Then Conjecture 3.7 holds.*

As we now show, if after adding an isolated node the  $\vartheta$ -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 5.17.

**Proposition 5.18.** *Let  $a \in \mathbb{N}$ . Assume that for all graphs  $G$  we have that  $\vartheta\text{-rank}(G \oplus i_0) \leq \vartheta\text{-rank}(G) + a$ . Then  $\vartheta\text{-rank}(G) \leq (a + 1)\alpha(G) - 1$  for all graphs  $G$ .*

PROOF. We proceed by induction on  $\alpha(G)$ . First, if  $\alpha(G) = 1$ , then  $\vartheta\text{-rank}(G) = 0 \leq a$ . Assume now  $\alpha(G) \geq 2$ . Using Proposition 5.16, and the assumption, we get  $\vartheta\text{-rank}(G) \leq a + 1 + \max_{i \in V} \vartheta\text{-rank}(G \setminus i^\perp)$ . Since  $\alpha(G \setminus i^\perp) \leq \alpha(G) - 1$ , we can apply the induction assumption to  $G \setminus i^\perp$  and obtain  $\vartheta\text{-rank}(G \setminus i^\perp) \leq (a + 1)(\alpha(G) - 1) - 1$ . This gives  $\vartheta\text{-rank}(G) \leq a + 1 + (a + 1)(\alpha(G) - 1) - 1 = (a + 1)\alpha(G) - 1$ .  $\square$

On the other hand, as we now show, the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence to  $\alpha(G)$  (i.e.,  $\vartheta$ -rank( $G$ ) is finite for all  $G$ ) if and only if the  $\vartheta$ -rank remains finite after adding an isolated node.

**Proposition 5.19.**  *$\vartheta^{(r)}(G)$  has finite convergence for every graph  $G$  if and only if  $\vartheta$ -rank( $G$ )  $< \infty$  implies  $\vartheta$ -rank( $G \oplus i_0$ )  $< \infty$ .*

PROOF. The ‘only if’ part is clear. We show the ‘if’ part by contradiction. So, assume that  $\vartheta$ -rank( $G$ )  $< \infty$  implies  $\vartheta$ -rank( $G \oplus i_0$ )  $< \infty$ . Assume also  $\vartheta^{(r)}(G)$  does not have finite convergence for some graph  $G$ . Assume, moreover, that  $G$  is a counterexample with the minimum number of nodes. By Proposition 5.16, we obtain that  $\vartheta$ -rank( $G \setminus i^\perp \oplus i$ ) =  $\infty$  for some  $i \in V$ . If  $i$  is not isolated in  $G$ , then  $G \setminus i^\perp \oplus i$  would be a counterexample with fewer nodes than  $G$ , contradicting the minimality of  $G$ . Hence,  $i$  is isolated in  $G$ , and thus we have  $G = (G \setminus i^\perp) \oplus i$ . Using again the minimality assumption, we know that  $\vartheta$ -rank( $G \setminus i^\perp$ )  $< \infty$ , which implies  $\vartheta$ -rank( $G$ ) =  $\vartheta$ -rank( $(G \setminus i^\perp) \oplus i$ )  $< \infty$ , thus yielding a contradiction.  $\square$

Clearly, if  $G$  has an isolated node  $i_0$ , then  $G \setminus i_0^\perp \oplus i_0 = G$  and thus the above result in Proposition 5.16 is of no use to derive information about the  $\vartheta$ -rank of  $G$  from the  $\vartheta$ -rank of the graphs  $G \setminus i^\perp \oplus i$ . This observation (already made in [GL07]) points out the difficulty of analyzing the  $\vartheta$ -rank of graphs with isolated nodes. We will investigate this question in Section 5.4.2 below.

On the other hand, adding an isolated node to a graph with  $\vartheta$ -rank = 0 preserves the property of having  $\vartheta$ -rank = 0, as observed in [GL07]. To see this, consider a graph  $G$  and set  $\alpha(G) = \alpha$ , so that  $\alpha(G \oplus i_0) = \alpha + 1$ . Then, we have

$$M_{G \oplus i_0} = \begin{pmatrix} \alpha & -1 \\ -1 & \frac{1}{\alpha} J \end{pmatrix} + \frac{\alpha + 1}{\alpha} \begin{pmatrix} 0 & 0 \\ 0 & \alpha(I + A_G) - J \end{pmatrix}, \quad (5.13)$$

where the blocks are indexed by  $i_0$  and  $V$  respectively. Then,  $M_{G \oplus i_0}$  belongs to  $\mathcal{K}_{n+1}^{(0)}$  if  $M_G \in \mathcal{K}_n^{(0)}$ . Indeed, the first matrix in the sum in (5.13) is positive semidefinite and the second one belongs to  $\mathcal{K}_{n+1}^{(0)}$  because adding a zero row/column preserves the cone  $\mathcal{K}^{(0)}$ . Observe that this decomposition is useless for analyzing the behavior of the  $\vartheta$ -rank after adding isolated nodes to graphs with  $\vartheta$ -rank at least one, because the second matrix on the right hand side does not belong to any cone  $\mathcal{K}_{n+1}^{(r)}$  if  $M_G \notin \mathcal{K}_n^{(0)}$  (recall Theorem 2.7).

Since adding an isolated node preserves the  $\vartheta$ -rank = 0 property, the next result follows as a direct application of Proposition 5.16.

**Lemma 5.20** ([dKP02]). *If  $\vartheta$ -rank( $G \setminus i^\perp$ ) = 0 for all  $i \in V$ , then we have  $\vartheta$ -rank( $G$ )  $\leq 1$ .*

**Example 5.21.** *As an application of Lemma 5.20 we obtain that*

$$\vartheta$$
-rank( $C_{2n+1}$ )  $\leq 1$  and  $\vartheta$ -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  $\vartheta$ -rank 0. Hence, by Lemma 5.20,  $\vartheta\text{-rank}(G) \leq 1$  and thus Conjecture 3.7 holds for graphs with  $\alpha(G) = 2$  (as shown in [dKP02]).

Let  $G = C_5 \oplus i_0$  be the graph obtained by adding one isolated node to the 5-cycle. As shown in [dKP02],  $G$  has  $\vartheta$ -rank 1 and the graph  $G \setminus i_0^\perp$  is the 5-cycle which also has  $\vartheta$ -rank 1. This shows that Lemma 5.20 does not permit to characterize, in general, graphs with  $\vartheta$ -rank 1. For details on the impact of adding isolated nodes to  $C_5$ , see Corollary 5.56.

As we will see in the next section, we can compute the  $\vartheta$ -rank of a more general class of graphs containing odd cycles and their complements.

**5.2.3.  $(\alpha, \omega)$ -graphs and critically imperfect graphs.** A graph  $G$  is called *critically imperfect* if it is not perfect and every induced subgraph  $H$  of  $G$  is perfect. For example, odd cycles of length at least 5, and their complements are critically imperfect. It was conjectured by Berge in [Ber61] that odd cycles (of length at least 5) and their complements are the only critically imperfect graphs. In 2006, Chudnovsky et. al [CRST06] show that this conjecture holds. This result is known as the Strong Perfect Graph Theorem and is one of the most celebrated results in graph theory in the last decades.

**Theorem 5.22.** [CRST06] *The only critically imperfect graphs are the odd cycles of length at least 5 and their complements.*

Earlier, in 1972, Lovász [Lov72] proved the following result known as the Perfect Graph Theorem: A graph  $G = (V, E)$  is perfect if and only if its complement  $\overline{G} = (V, \overline{E})$  is perfect. Additionally, in the attempt of showing the Strong Perfect Graph Theorem (Conjecture back then), Lovász defined the notion of  $(\alpha, \omega)$ -graphs, and showed that every critically imperfect graph is an  $(\alpha, \omega)$ -graph. A graph  $G = (V, E)$  with  $|V| = \alpha\omega + 1$  is an  $(\alpha, \omega)$ -graph if, for every vertex  $v$ , the vertices of  $G \setminus v$  can be partitioned into  $\alpha$  cliques of size  $\omega$ , and into  $\omega$  independent sets of size  $\alpha$ .

In general, there are many  $(\alpha, \omega)$ -graphs that are not critically imperfect. However, in [Lov83], Lovász pointed out that critically imperfect graphs and  $(\alpha, \omega)$ -graphs satisfy many similar properties: he wrote

*“it seems that virtually all the structural results which we know for critically imperfect graphs also follow for  $(\alpha, \omega)$ -graphs. This indicates the main difficulty in the proof of the Strong Perfect Graph Conjecture - it is difficult to determine that an  $(\alpha, \omega)$ -graph is not critically imperfect”.*

This motivates us to study the  $\vartheta$ -rank for  $(\alpha, \omega)$ -graphs, as an attempt to

possibly find properties that separate critically imperfect graphs from  $(\alpha, \omega)$ -graphs. Unfortunately, this attempt fails since we can show that every  $(\alpha, \omega)$ -graph has  $\vartheta$ -rank 1 (see Theorem 5.24 below). In what follows we show this result.

For showing that  $\vartheta\text{-rank}(G) = 1$ , we shall prove that  $\vartheta^{(0)}(G) > \alpha(G)$  and that  $\vartheta^{(1)}(G) = \alpha(G)$ . Lovász [Lov83] showed that  $\vartheta(G) > \alpha(G)$  for every  $(\alpha, \omega)$ -graph  $G$ . Ahmadi and Dibek [AD2022] observed that the proof of Lovász can be extended to the parameter  $\vartheta'$ , thus showing that  $\vartheta'(G) = \vartheta^{(0)}(G) > \alpha(G)$  for  $(\alpha, \omega)$ -graphs. We give a new proof of this known fact using the properties of the  $\mathcal{K}^{(0)}$ -certificates developed in Section 5.1 (see Proof of Theorem 5.24). On the other hand, we use Lemma 5.20 for showing that  $\vartheta\text{-rank}(G) \leq 1$  for every  $(\alpha, \omega)$ -graph  $G$ .

We recall some structural properties of  $(\alpha, \omega)$ -graphs that will be useful for showing Theorem 5.24 below. It was shown by Lovász [Lov83] that if  $G$  is an  $(\alpha, \omega)$ -graph, then  $\alpha(G) = \alpha$  and  $\omega(G) = \omega$ . Moreover, we have the following result.

**Theorem 5.23** (Lovász [Lov83]). *Let  $G$  be an  $(\alpha, \omega)$ -graph with  $|V| = n$ . Then, the following assertions hold.*

- (i)  $G$  has exactly  $n$  cliques of size  $\omega$ .
- (ii)  $G$  has exactly  $n$  stable sets of size  $\alpha$ .
- (iii) Every vertex is in exactly  $\omega$  cliques of size  $\omega$ .
- (iv) Every vertex is in exactly  $\alpha$  stable sets of size  $\alpha$ .
- (v) Every independent set of size  $\alpha$  is disjoint from exactly one clique of size  $\omega$ .

Now we can show the following result.

**Theorem 5.24.** *Let  $G$  be an  $(\alpha, \omega)$ -graph, then  $\vartheta\text{-rank}(G) = 1$ .*

PROOF. We first show that  $\vartheta\text{-rank}(G) \leq 1$ . For this, we show that  $\vartheta\text{-rank}(G \setminus i^\perp) = 0$  for every  $i \in V$ , and use Lemma 5.20. Let  $i \in V$ . It is easy to observe from the definition that no vertex in an  $(\alpha, \omega)$ -graph is isolated, so there exists  $j \in N_G(i)$ . Since  $G$  is an  $(\alpha, \omega)$ -graph, the vertices of  $G \setminus j$  can be partitioned into  $\alpha$  cliques  $C_1, C_2, \dots, C_\alpha$ . Assume  $i \in C_1$ . Then, the vertices of  $G \setminus i^\perp$  can be partitioned by the  $\alpha(G) - 1$  cliques  $C_2, C_3, \dots, C_\alpha$ . Since every vertex belongs to a stable set of size  $\alpha$  (see Theorem 5.23), then  $\alpha(G \setminus i^\perp) = \alpha(G) - 1$ . This shows that  $\alpha(G \setminus i^\perp) = \bar{\chi}(G \setminus i^\perp)$ , and thus  $\vartheta\text{-rank}(G \setminus i^\perp) = 0$ .

We show now that  $\vartheta\text{-rank}(G) > 0$  i.e.,  $\vartheta^{(0)}(G) > \alpha(G)^1$ . Assume by contradiction that  $\vartheta\text{-rank}(G) = 0$ , i.e.,  $M_G \in \mathcal{K}_n^{(0)}$ . Let  $P$  be a  $\mathcal{K}^{(0)}$ -certificate

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<sup>1</sup>This fact was already proved in [AD2022]. We give a new proof.

for  $M_G$ . For any stable set  $S$  of size  $\alpha$  we have that  $(\chi^S)^\top M_G \chi^S = 0$  (recall relation (5.9)). Then, by Lemma 5.3,  $\chi^S \in \ker P$  for any stable set  $S$  of size  $\alpha$ . Therefore,

$$\sum_{\substack{S \text{ is stable} \\ |S|=\alpha}} \chi^S \in \ker P.$$

By Theorem 5.23 (iv), every vertex belongs to exactly  $\alpha$  stable sets of size  $\alpha$ . Hence,

$$\frac{1}{\alpha} \cdot \sum_{\substack{S \text{ is stable} \\ |S|=\alpha}} \chi^S = e \in \ker P.$$

By definition of  $(\alpha, \omega)$ -graphs, for any  $i \in V$ , the vertices of  $G \setminus i$  can be partitioned into  $\omega$  stable sets  $S_1, S_2, \dots, S_\omega$  of size  $\alpha$ . Then, we have

$$\chi^{S_1} + \chi^{S_2} + \dots + \chi^{S_\omega} = e - \chi^{\{i\}} \in \ker P.$$

This, combined with the fact that  $e \in \ker P$ , shows that  $\chi^{\{i\}} = e_i \in \ker P$  for every vertex  $i$ . Hence, the matrix  $P$  is the zero matrix. Since  $P$  is  $\mathcal{K}^{(0)}$ -certificate for  $M_G$ , we have  $P \leq M_G$ . Then,  $G$  is a complete graph, which yields a contradiction.  $\square$

### 5.3. Towards characterizing graphs with $\vartheta$ -rank 0

In this section, we investigate the graphs  $G$  with  $\vartheta$ -rank 0, i.e., such that  $\vartheta^{(0)}(G) = \alpha(G)$  or, equivalently,  $M_G \in \mathcal{K}_n^{(0)}$ . Recall the well-known ‘sandwich inequality’ from [Lov79] (see also Chapter 3):

$$\alpha(G) \leq \vartheta'(G) = \vartheta^{(0)}(G) \leq \vartheta(G) \leq \bar{\chi}(G). \quad (5.14)$$

If  $G$  can be covered by  $\alpha(G)$  cliques (i.e.,  $\bar{\chi}(G) = \alpha(G)$ ), then  $G$  has  $\vartheta$ -rank 0. In addition, if  $\alpha(G) = \alpha$  and  $V_1, V_2, \dots, V_\alpha$  are cliques partitioning  $V$ , then the matrix

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

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 for graphs with  $\alpha(G) \leq 2$ . We also provide an algorithmic method that permits to reduce the characterization of  $\vartheta$ -rank 0 graphs to the same property for the class of acritical graphs.

Throughout we often set  $\alpha := \alpha(G)$  to simplify notation.

**5.3.1. Characterizing critical graphs with  $\vartheta$ -rank 0.** The next result will be repeatedly used.

**Lemma 5.25.** *Let  $G$  be a graph with  $\alpha(G) = \alpha$  and let  $S$  be an  $\alpha$ -stable set. Assume  $M_G \in \mathcal{K}_n^{(0)}$  and let  $P$  be a  $\mathcal{K}^{(0)}$ -certificate for  $M_G$ . Then,  $\chi^S \in \ker(P)$  and  $P[S] = \alpha I_\alpha - J_\alpha$ .*

PROOF. Directly from Lemma 5.3 (recall relation (5.9)).  $\square$

**Proposition 5.26.** *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  $\vartheta$ -rank( $G$ ) = 0, then each connected component of the graph  $G_c$  is a clique of  $G$ .*

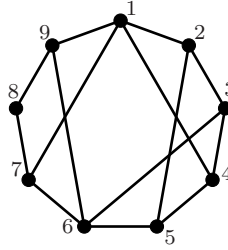
PROOF. By assumption,  $\vartheta$ -rank( $G$ ) = 0. Let  $P$  be a  $\mathcal{K}^{(0)}$ -certificate for  $M_G$ . Let  $V_1, V_2, \dots, V_p$  be the connected components of the graph  $G_c$ . We show that each component  $V_i$  is a clique in  $G$ . For this, pick two nodes  $u \neq v \in V_i$  that 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  $\alpha$ -stable in  $G$ . Then, by Lemma 5.25, the characteristic vectors  $\chi^{I \cup \{u\}}$  and  $\chi^{I \cup \{v\}}$  both belong to the kernel of  $P$  and thus  $\chi^{\{u\}} - \chi^{\{v\}} \in \ker P$ . From this, we deduce that the columns of  $P$  indexed by the nodes in  $V_i$  are all equal. Combining this with the fact that the diagonal entries of  $P$  are equal to  $\alpha - 1$  and that  $P$  is symmetric we can conclude that, with respect to the partition  $V = V_1 \cup \dots \cup V_p$ , the matrix  $P$  has the following block-form:

$$P = \begin{pmatrix} (\alpha - 1)J_{|V_1|} & a_{12}J_{|V_1| \times |V_2|} & \cdots & a_{1p}J_{|V_1| \times |V_p|} \\ a_{21}J_{|V_2| \times |V_1|} & (\alpha - 1)J_{|V_2|} & \cdots & a_{2p}J_{|V_2| \times |V_p|} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1}J_{|V_p| \times |V_1|} & a_{p2}J_{|V_p| \times |V_2|} & \cdots & (\alpha - 1)J_{|V_p|} \end{pmatrix} \quad (5.15)$$

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

**Corollary 5.27.** *Assume  $G = (V, E)$  is a critical graph, i.e., all its edges are critical. Then, we have  $\vartheta$ -rank( $G$ ) = 0 if and only if  $G$  is the disjoint union of  $\alpha(G)$  cliques. In particular, we have  $\vartheta$ -rank( $G$ ) = 0 if and only if  $\bar{\chi}(G) = \alpha(G)$ .*

PROOF. The ‘only if’ part follows from Proposition 5.26 and the ‘if part’ follows from relation (5.14). The last claim follows directly.  $\square$

FIGURE 5.3. Graph  $H_9$ , acritical

In Theorem 5.24, we show that every  $(\alpha, \omega)$ -graph has  $\vartheta$ -rank 1. In particular, odd cycles and their complements have  $\vartheta$ -rank 1. This last claim was already shown in [PVZ07]. We give a new proof of this last fact using Proposition 5.26 and Corollary 5.27.

**Example 5.28.** Let  $n \geq 2$ . We saw in Example 5.21 that  $\vartheta\text{-rank}(C_{2n+1}) \leq 1$  and  $\vartheta\text{-rank}(\overline{C_{2n+1}}) \leq 1$ . Here, we can show that their  $\vartheta$ -rank is equal 1.

- (i)  $C_{2n+1}$  is critical and connected (and not a clique) and thus, by Corollary 5.27,  $\vartheta\text{-rank}(C_{2n+1}) \geq 1$ .
- (ii) The critical edges of the graph  $G = \overline{C_{2n+1}}$  are those of the form  $\{i, i+2\}$  (for  $i \in [2n+1]$ , indices taken modulo  $2n+1$ ). Hence, the subgraph  $G_c$  (of critical edges) is connected (and not a clique) and thus  $\vartheta\text{-rank}(\overline{C_{2n+1}}) \geq 1$ .

Observe that this gives an alternative proof for the fact that  $H \in \mathcal{K}_5^{(1)} \setminus \mathcal{K}_5^{(0)}$ , using that  $H = M_{C_5}$ .

Next, we give an example of an acritical graph with  $\vartheta$ -rank 1.

**Example 5.29.** Consider the graph  $H_9$  from Figure 5.3. 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 5.11,  $\vartheta\text{-rank}(H_9) \leq \vartheta\text{-rank}(C_9) = 1$ .

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 4 in  $H_9$ , by applying Lemma 5.25 we obtain

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

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

**5.3.2. Characterizing graphs with  $\alpha(G) = 2$  and  $\vartheta\text{-rank}(G) = 0$ .** Here, we observe that the result of Corollary 5.27 holds for all (not necessarily critical) graphs with  $\alpha(G) \leq 2$ .

**Lemma 5.30.** *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  $\vartheta\text{-rank}(G) = 0$ . Let  $P$  be a  $\mathcal{K}^{(0)}$ -certificate for  $M_G$ , i.e.,  $P \succeq 0$ ,  $M_G \geq P$  and  $P_{ii} = \alpha(G) - 1 = 1$  for all  $i \in V$ . As  $P \succeq 0$  with diagonal entries equal to 1 it follows that  $-1 \leq P_{ij} \leq 1$  for all  $i, j \in V$ . On the other hand,  $P \leq M_G$  implies  $P_{ij} \leq -1$  for all positions corresponding to non-edges. Therefore we have  $P_{ij} = -1$  for every non-edge  $\{i, j\}$ .

As  $P \succeq 0$  we may assume that  $P$  is the Gram matrix of unit vectors  $v_1, \dots, v_n \in \mathbb{R}^n$ , i.e.,  $P = (v_i^T v_j)_{i, j \in V}$ . Then, for any two non-adjacent vertices  $i, j$ , we have  $v_i^T v_j = -1$  and thus  $v_i = -v_j$ . Pick a unit vector  $r \in \mathbb{R}^n$  such that  $r^T v_i \neq 0$  for all  $i \in V$  (such a vector exists since the kernel of  $P$  is nontrivial by Lemma 5.25). Define the sets  $V_1 = \{i \in V : r^T v_i > 0\}$  and  $V_2 = \{i \in V : r^T v_i < 0\}$ . Then  $V_1$  and  $V_2$  are two cliques of  $G$  that cover  $V$ .  $\square$

**Example 5.31.** *We give some examples showing that the characterization in Corollary 5.27 and Lemma 5.30 of  $\vartheta\text{-rank} 0$  graphs as those with  $\bar{\chi}(G) = \alpha(G)$  does not hold if  $\alpha(G) \geq 3$  and  $G$  has some non-critical edges.*

Let  $G$  be the Petersen graph. Then  $G$  has rank 0, since  $\vartheta(G) = \vartheta^{(0)}(G) = \alpha(G) (= 4)$ , but  $\bar{\chi}(G) = 5 > \alpha(G) = 4$  (see [Lov79]). Note that the Petersen graph is in fact acritical. The graph  $G = \overline{G_{13}}$  considered in [MR16] provides another example with  $3 = \alpha(G) = \vartheta^{(0)}(G) < \bar{\chi}(G) = 4$  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  $G_{n,k}$  has as vertex set the collection of all  $k$ -subsets of  $[n]$ , where two vertices are adjacent if the corresponding subsets are disjoint. Note that  $G_{5,2}$  is the Petersen graph. It has been shown by Lovász [Lov79, LK78] that

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

Therefore,  $\vartheta\text{-rank}(G_{n,k}) = 0$ . However,  $\bar{\chi}(G_{n,k}) \geq \binom{n}{k} / \lfloor n/k \rfloor > \binom{n-1}{k-1} = \alpha(G_{n,k})$  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. [Erd61] who proved that for  $n > 2k$  the maximum stable sets of the Kneser graph  $G_{n,k}$  are of the form  $\mathcal{A}_j := \{S \subseteq [n] : j \in S, |S| = k\}$  for  $j \in [n]$ . To see that  $G_{n,k}$  is acritical, assume, for contradiction, that  $\{A, B\}$  is a critical edge. Then, there exists a collection  $\mathcal{I}$  of  $k$ -subsets of  $[n]$  such that  $\mathcal{I} \cup \{A\} = \mathcal{A}_i$  and  $\mathcal{I} \cup \{B\} = \mathcal{A}_j$  for  $i \neq j \in [n]$ . Hence, every element



of  $\mathcal{I}$  contains both  $i$  and  $j$ , so that  $|\mathcal{I}| \leq \binom{n-2}{k-2}$ . This gives a contradiction as  $|\mathcal{I}| + 1 = |\mathcal{A}_j| = \binom{n-1}{k-1}$ .

### 5.3.3. Reduction of $\vartheta$ -rank 0 graphs to the class of acritical graphs.

Here, we further investigate the structure of graphs with  $\vartheta$ -rank 0. We introduce a reduction procedure, which we use to reduce the task of checking the  $\vartheta$ -rank 0 property to the same property for the class of acritical graphs. This procedure relies on the following graph construction, which is motivated by Proposition 5.26.

**Definition 5.32.** 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  $\vartheta$ -rank 0 property and the stability number.

**Lemma 5.33.** Assume  $G$  is a graph with  $\vartheta\text{-rank}(G) = 0$  and let  $\Gamma(G)$  be the graph as in Definition 5.32. 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  $\alpha$ -stable set in  $G$  and, for each  $v \in S$ , let  $V_v$  denote the connected component of  $G_c$  that contains  $v$ . Since each  $V_i$  is a clique of  $G$  (by Lemma 5.26), 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  $\alpha$  in  $\Gamma(G)$ .

Next, we show that  $\vartheta\text{-rank}(\Gamma(G)) = 0$ . By assumption,  $\vartheta\text{-rank}(G) = 0$  and thus  $M_G = P + N$ , where  $P \succeq 0$ ,  $N \geq 0$  and  $P_{ii} = \alpha - 1$  for all  $i \in V$ . As shown in the proof of Lemma 5.26, the matrix  $P$  has the block-form (5.15) with respect to the partition  $V = V_1 \cup \dots \cup V_p$ . Then the following  $p \times p$  matrix

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

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

Finally, we prove  $\alpha(\Gamma(G)) \leq \alpha$ . For this, let  $I \subseteq [p]$  be an  $\alpha(\Gamma(G))$ -stable set. For any  $i \neq j \in I$  the set  $V_i \cup V_j$  is not a clique in  $G$  and thus  $a_{ij} \leq -1$

(as observed above). Consider the principal submatrix  $P'[I]$  of  $P'$  indexed by  $I$ . Then, we have

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

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

**Lemma 5.34.** *Assume  $\vartheta$ -rank( $G$ ) = 0. Then we have  $\bar{\chi}(\Gamma(G)) \geq \bar{\chi}(G)$ . In particular, if  $\Gamma(G)$  is covered by  $\alpha(\Gamma(G))$  cliques, then  $G$  is covered by  $\alpha(G)$  cliques.*

PROOF. If  $C \subseteq [p]$  is a clique of  $\Gamma(G)$ , then  $\bigcup_{i \in C} C_i$  is a clique in  $G$ . Therefore, if we can cover  $V(\Gamma(G)) = [p]$  by  $k$  cliques of  $\Gamma(G)$ , then we can cover  $V(G)$  by  $k$  cliques of  $G$ . The last claim follows from the fact that  $\alpha(\Gamma(G)) = \alpha(G)$  (Lemma 5.33).  $\square$

Now, we provide a partial converse to the result of Lemma 5.33.

**Lemma 5.35.** *Let  $G = (V, E)$  be a graph and let  $G_c = (V, E_c)$  be its subgraph of critical edges. Assume that the connected components  $V_1, \dots, V_p$  of  $G_c$  are cliques in  $G$  and let  $\Gamma(G)$  be as in Definition 5.32. If  $\vartheta$ -rank( $\Gamma(G)$ ) = 0 and  $\alpha(\Gamma(G)) \leq \alpha(G)$ , then we have  $\vartheta$ -rank( $G$ ) = 0.*

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

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

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

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

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

So, we have shown that if we apply the  $\Gamma$ -operator to a graph  $G$  with  $\vartheta$ -rank 0, then we obtain a new graph  $\Gamma(G)$  with  $\vartheta$ -rank 0, with the same stability number and with  $|V(\Gamma(G))| \leq |V(G)|$ , where the inequality is strict

if  $G$  has critical edges. We may iterate this construction until obtaining a graph without critical edges.

**Definition 5.36.** *Let  $G$  be a graph with  $\vartheta$ -rank( $G$ ) = 0. We define the residual graph  $R(G)$  of  $G$  as the graph  $\Gamma^k(G)$ , where  $k$  is the smallest integer such that  $\Gamma^k(G)$  has no critical edge, after setting  $\Gamma^{i+1}(G) = \Gamma(\Gamma^i(G))$  for any  $i \geq 0$ .*

As a direct application of Lemmas 5.33 and 5.34 we obtain the following result.

**Lemma 5.37.** *Let  $G$  be a graph with  $\vartheta$ -rank( $G$ ) = 0 and let  $R(G)$  be its residual graph as defined in Definition 5.36. Then,  $R(G)$  has no critical edges and we have  $\vartheta$ -rank( $R(G)$ ) = 0,  $\alpha(R(G)) = \alpha(G)$ , and  $\bar{\chi}(R(G)) \geq \bar{\chi}(G)$ .*

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

**Algorithm:** REDUCE-TO-ACRITICAL

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

**Output:** Either:  $\vartheta$ -rank( $G$ )  $\geq 1$ . Or: the graph  $R(G)$ , which is acritical with  $\alpha(R(G)) = \alpha(G)$  and such that  $\vartheta$ -rank( $G$ ) = 0  $\iff$   $\vartheta$ -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:**  $\vartheta$ -rank( $G$ )  $\geq 1$ .
- (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:**  $\vartheta$ -rank( $G$ )  $\geq 1$ .
- (4) If  $\Gamma(G)$  is acritical then **return:**  $\Gamma(G)$ . Otherwise, set  $G = \Gamma(G)$  and go to Step 1.

We verify the correctness of the output of the above algorithm. For this, let us assume the algorithm does not output  $\vartheta$ -rank( $G$ )  $\geq 1$ . In view of Definition 5.36, the returned graph at step 4 is the residual graph  $R(G)$ , which is acritical by construction. In addition, in view of Step 3, we have  $\alpha(R(G)) = \alpha(G)$ . Remains to check that  $\vartheta$ -rank( $G$ ) = 0 if and only if  $\vartheta$ -rank( $R(G)$ ) = 0. Indeed, the ‘only if’ part follows using iteratively Lemma 5.33, and the ‘if part’ follows using Lemma 5.35.

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

**Theorem 5.38.** *For any fixed integer  $\alpha$ , the problem of deciding whether a graph with stability number  $\alpha$  has  $\vartheta$ -rank 0 is reducible in polynomial time to the problem of deciding whether a graph with no critical edges and stability number  $\alpha$  has  $\vartheta$ -rank 0.*

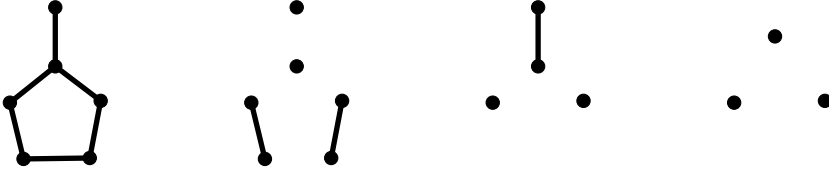


FIGURE 5.4. From right to left, the graphs  $G$ ,  $G_c$  (consisting of the critical edges of  $G$ ),  $\Gamma(G)$ ,  $R(G) = \Gamma^2(G)$

**Example 5.39.** We illustrate in Figure 5.4 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,  $\vartheta\text{-rank}(R(G)) = 0$ , which shows again  $\vartheta\text{-rank}(G) = 0$ .

**Remark 5.40.** The results from this section can be adapted to the Lovász parameter  $\vartheta(G)$  instead of  $\vartheta^{(0)}(G)$ . Recall from [Lov79] 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 ‘ $\vartheta\text{-rank}(G) = 0$ ’ 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  $\alpha$  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.

**5.3.4. Acritical graphs with large stability number and  $\vartheta$ -rank 0.**

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

**Proposition 5.41.** 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  $\vartheta\text{-rank}(G) = 0$ .
- (ii) If  $\alpha(G) = |V| - 3$ , then  $\overline{\chi}(G) = \alpha(G)$  and thus  $\vartheta\text{-rank}(G) = 0$ , unless  $G$  is the disjoint union of  $C_5$  and isolated nodes in which case  $\vartheta\text{-rank}(G) \geq 1$  and  $G$  is critical.
- (iii) If  $\alpha(G) = |V| - 4$  and  $G$  is acritical, then  $\overline{\chi}(G) = \alpha(G)$  and thus  $\vartheta\text{-rank}(G) = 0$ .

PROOF. Throughout we set  $\alpha = \alpha(G)$ . We will 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  $n = |V|$ .

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

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

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

Let  $S$  be an  $\alpha$ -stable set and set  $V \setminus S = \{x, y, z\}$ . Assume  $G$  is not covered by  $\alpha$  cliques, 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  $\alpha(H) \geq \underline{2k - 2}$ . 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  $\alpha$  cliques, which we had excluded. Therefore, one must have  $N_S(\{x, y, z\}) = \{u, w\}$ , which implies that  $G$  is  $C_5$  together with  $n - 5$  isolated nodes.

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

Let  $S$  be an  $\alpha$ -stable set and set  $T = \{x, y, z, w\} = V \setminus S$ . Note that every vertex of  $T$  has at least two neighbors in  $S$ , otherwise the edge between that vertex and  $S$  would be a critical edge of  $G$ . In addition, if there is a matching between  $T$  and  $S$  that covers all the nodes in  $T$ , then  $V$  is covered by  $\alpha$  cliques (the four edges of the matching and the remaining  $\alpha - 4$  vertices in  $S$ ) and we are done. Hence, we may now assume that there is no matching between  $S$  and  $T$  that covers  $T$ . By Hall's theorem (see [Hall35]), there exists  $W \subseteq T$  such that  $|N_S(W)| \leq |W| - 1$ . Then,  $|W| \geq 3$  since  $|N_S(W)| \geq 2$ . We distinguish two cases.

**Case 3a:** First, assume  $|W| = 3$ , say  $W = \{x, y, z\}$ . Then  $|N_S(W)| = 2$ , say  $N_S(W) = \{u, v\}$ . So,  $N_S(x) = N_S(y) = N_S(z) = \{u, v\}$ . Since the set  $(S \setminus \{u, v\}) \cup \{x, y, z\}$  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 3 (say,  $\{x, y, z\}$ ) and (ii) when  $T$  contains two disjoint edges (say,  $\{x, y\}, \{z, w\} \in E$ ) since then  $G$  is covered by the cliques  $\{x, y, z, u\}$ ,  $\{v, w\}$  in case (i), or  $\{x, y, u\}$ ,  $\{z, w, v\}$  in case (ii), and the  $\alpha - 2$  singletons in  $S \setminus \{u, v\}$ . So we may now assume that  $T$  does not contain a triangle nor two disjoint edges. But then we reach a contradiction with the fact that each of the two sets  $S \setminus \{u, v\} \cup \{x, z, w\}$  and  $S \setminus \{u, v\} \cup \{y, z, w\}$  is not a stable set and thus contains an edge.

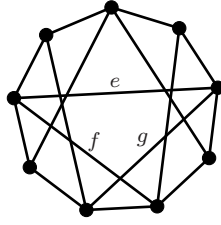


FIGURE 5.5. Graph  $G_9$  has  $\alpha(G_9) = 4$ ,  $\vartheta(G_9) = \vartheta^{(0)}(G_9) = 4.155$ ,  $\bar{\chi}(G_9) = 5$

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

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

**Remark 5.42.** (i) As we just saw in Proposition 5.41 (ii), the only graphs  $G$  with  $\alpha(G) = |V| - 3$  that do not have  $\vartheta$ -rank 0 are of the form  $G = C_5 \oplus \overline{K_{n-5}}$ , the disjoint union of  $C_5$  and  $n - 5$  isolated nodes. In fact, we will show that  $\vartheta\text{-rank}(C_5 \oplus \overline{K_{n-5}}) = 1$  if and only if  $n \leq 13$  (see Corollary 5.56 in Section 5.4.2).

(ii) Proposition 5.41 shows that any acritical graph for which we have  $\alpha(G) \geq |V| - 4$  satisfies  $\bar{\chi}(G) = \alpha(G)$  and thus has  $\vartheta$ -rank 0. The same holds for graphs with  $\alpha(G) = 2$  (Lemma 5.30). The next natural case to consider are graphs with  $\alpha(G) = 3$  and  $n \geq 8$  nodes. Polak

[Pol21] verified (using computer) that if  $G$  is an acritical graph on 8 nodes with  $\alpha(G) = 3$ , then  $\bar{\chi}(G) = \alpha(G)$  holds (and thus  $\vartheta\text{-rank}(G) = 0$ ). In addition, if  $G$  is acritical on 9 nodes with  $\alpha(G) = 3$ , then  $\vartheta\text{-rank}(G) = 0$  holds as well (but sometimes with  $\bar{\chi}(G) > \alpha(G)$ ). On the other hand, there exist acritical graphs on  $n = 10$  nodes with  $\alpha(G) = 3$  that do not have  $\vartheta\text{-rank} 0$ .

- (iii) There are acritical graphs  $G$  with  $4 \leq \alpha(G) \leq |V| - 5$  that cannot be covered by  $\alpha(G)$  cliques. As a first example, consider the graph  $G_9$  in Figure 5.5, which is acritical, with  $|V| = 9$ ,  $\alpha(G_9) = 4$ ,  $\bar{\chi}(G_9) = 5$ , and  $\vartheta(G_9) = \vartheta^{(0)}(G_9) = 4.155$ , and thus  $\vartheta\text{-rank}(G_9) \geq 1$ . Moreover, with  $e, f, g$  being the three labeled edges in  $G_9$ , each of the three graphs  $G_9 \setminus e$ ,  $G_9 \setminus \{f, g\}$  and  $G_9 \setminus \{e, f\}$  is acritical and satisfies  $\vartheta^{(0)}(G) = \vartheta(G) > \alpha(G)$ . This gives four non-isomorphic acritical graphs on 9 vertices that have  $\vartheta\text{-rank}$  at least 1 (and thus cannot be covered by  $\alpha(G)$  cliques). Polak [Pol21] verified (using computer) that these are the only non-isomorphic acritical graphs on 9 vertices that do not have  $\vartheta\text{-rank} 0$ .
- (iv) Finally, we use the graph  $H_9$  from Example 5.29 to construct a class of acritical graphs with  $\bar{\chi}(G) > \alpha(G)$  and  $\vartheta\text{-rank}(G) \geq 1$ . For any pair  $(n, \alpha)$  with  $4 \leq \alpha \leq n - 5$ , we construct an acritical graph  $G$  on  $n$  nodes with  $\alpha(G) = \alpha$  and  $\bar{\chi}(G) > \alpha(G)$ . For this, we let the vertex set of  $G$  be partitioned as  $V = V_0 \cup V_1 \cup V_2$ , where  $|V_0| = 9$ ,  $|V_1| = n - 5 - \alpha$  and  $|V_2| = \alpha - 4$ , and we select the following edges: on  $V_0$  we put a copy of  $H_9$ , on  $V_1$  we put a clique, we let every node of  $V_1$  be adjacent to every node of  $V_0$ , and we let  $V_2$  consist of isolated nodes. Then, it is easy to see that  $\alpha(G) = \alpha$ ,  $G$  is acritical and  $\bar{\chi}(G) > \alpha(G)$ . One can show that  $\vartheta\text{-rank}(G) = \vartheta\text{-rank}(H_9 \oplus \overline{K_{\alpha-4}})$ . This follows from the following (easy-to-check) property: If  $\{i, j\}$  is an edge and  $N(i) \subseteq N(j)$  then  $\vartheta\text{-rank}(G \setminus j) = \vartheta\text{-rank}(G)$ . Since  $\vartheta\text{-rank}(H_9) = 1$  one can now deduce that  $\vartheta\text{-rank}(G) \geq 1$ .

#### 5.4. On the impact of isolated nodes on the $\vartheta$ -rank

As mentioned in Proposition 5.17, if the  $\vartheta$ -rank does not increase under the simple graph operation of adding an isolated node, then Conjecture 3.7 holds. In [GL07] it was conjectured that adding isolated nodes indeed does not increase the  $\vartheta$ -rank. In this section, we investigate this question and in fact disprove the latter conjecture, already for graphs with  $\vartheta$ -rank 1. For this, we first observe that critical edges provide a lot of structure on the matrices  $P(i)$  ( $i \in V$ ) appearing in  $\mathcal{K}^{(1)}$ -certificates, which can be exploited for verifying whether a graph has  $\vartheta$ -rank 1.

We investigate the impact of adding isolated nodes to certain classes of graphs  $H$  with  $\vartheta$ -rank 1. First, when the subgraph of critical edges of  $H$

is connected, we give an upper bound on the number of isolated nodes that can be added to  $H$  while preserving the  $\vartheta$ -rank 1 property (Theorem 5.48). Second, we show that adding this number of isolated nodes indeed produces a graph with  $\vartheta$ -rank 1 when  $H$  satisfies the property  $\vartheta\text{-rank}(H \setminus i^\perp) = 0$  for all its nodes (Theorem 5.55). As an application, we are able to determine the exact number of isolated nodes that can be added to an odd cycle  $C_{2n+1}$  ( $n \geq 2$ ) or its complement while preserving the  $\vartheta$ -rank 1 property (see Corollary 5.56). As a byproduct, we obtain that adding an isolated node to a graph with  $\vartheta$ -rank 1 can produce a graph with  $\vartheta$ -rank  $\geq 2$ . For instance,  $C_5 \oplus \overline{K_8}$  has  $\vartheta$ -rank 1, but  $C_5 \oplus \overline{K_9}$  has  $\vartheta$ -rank 2.

**5.4.1. Properties of the kernel of  $\mathcal{K}^{(1)}$ -certificates.** We first investigate properties on the  $\mathcal{K}^{(1)}$ -certificates applied to the matrices  $M_G$ . The following results are based on the kernel property shown in Lemma 5.4.

**Lemma 5.43.** *Let  $G = (V = [n], E)$  be a graph with  $\vartheta\text{-rank}(G) = 1$ . Let  $\{P(j) : j \in V\}$  be a  $\mathcal{K}^{(1)}$ -certificate for  $M_G$ , let  $i \in V$  and let  $C_1, C_2, \dots, C_n$  denote the columns of the matrix  $P(i)$ . Then the following holds.*

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

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

$$P(i) = \left( \begin{array}{c|c} (\alpha - 1)J_{|i^\perp|} & -1 \\ \hline -1 & \frac{1}{\alpha - 1}J_{|V \setminus i^\perp|} \end{array} \right), \quad (5.16)$$

*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 5.4 (i), which claims  $P(i)x = 0$  as  $x^T M_G x = 0$  for  $x = \chi^S$ .

We now show part (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  $\alpha$ -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 relation (5.8) and Theorem 5.7). Using Lemma 5.4 (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  $C_i = C_j$ .

Finally, we show part (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  $\alpha$  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  $\alpha$ -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



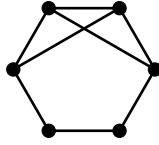


FIGURE 5.6. A critical graph with stability number 2

$C_l = C_m$  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  $\alpha$ -stable set of the form  $\{i\} \cup I$  (with  $I \subseteq V \setminus i^\perp$ ) we have  $C_i + \sum_{k \in I} C_k = 0$  which, combined with the fact that  $P(i)_{ii} = \alpha - 1$ , implies the desired structure for the matrix  $P(i)$ .  $\square$

Using Lemma 5.43, we can show that for some  $\vartheta$ -rank 1 graphs, the construction of the matrices  $P(i)$  in a  $\mathcal{K}^{(1)}$ -certificate is, in fact, unique. We already saw that this is the case for the 5-cycle in Example 5.5, 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 5.6 an example of a critical graph with stability number  $\alpha(G) = 2$ ; of course,  $C_5$  is another such example.

**Example 5.44.** Let  $G = (V, E)$  be a critical graph with  $\alpha(G) = 2$ . Then,  $M_G \in \mathcal{K}^{(1)}$  (recall Theorem 5.14). Let  $\{P(i) : i \in V\}$  be a  $\mathcal{K}^{(1)}$ -certificate for  $M_G$ . We show that the matrices  $P(i)$  are uniquely determined using Lemma 5.16. 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 5.43 can be applied and we obtain that for every  $i \in V$  the matrix  $P(i)$  takes the form (5.16).

**Example 5.45.** 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 5.43 we conclude that the matrix  $P(i_0)$  takes the form (5.16) (also displayed below). In particular, we have  $P(i_0)_{ij} = 1/2$  and  $P(i_0)_{i_0i} = -1$  for all  $i, j \in [5]$ . We now show that for any  $i \in [5]$  also the matrices  $P(i)$  are uniquely determined; by symmetry, it suffices to show this for matrix  $P(1)$ .

Since  $G$  is critical, by Lemma 5.43 (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 5.43 (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 5.1, 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 5.43(i) we obtain that the columns indexed by 1, 3 and  $i_0$  sum up to

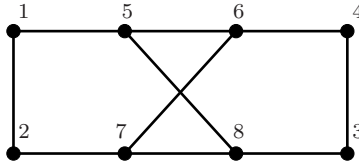


FIGURE 5.7. The graph  $G_8$  (critical,  $\alpha(G_8) = 3$ )

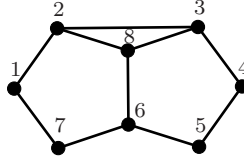


FIGURE 5.8. The graph  $H_8$  (critical,  $\alpha(H_8) = 3$ )

0, which enables us to complete the rest of the matrix  $P(1)$ , whose shape is shown below.

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

**Lemma 5.46.** 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 5.7 there exists  $x \in \Delta_n$  such that  $x^T M_G x = 0$  and  $\text{Supp}(x) = S$ . Then Lemma 5.4 (ii) gives the desired result.  $\square$

**Example 5.47.** Consider the graph  $G_8$  shown in Figure 5.7, which is critical with  $\alpha(G_8) = 3$ . We show that  $\vartheta\text{-rank}(G_8) \geq 2$  (which was verified numerically in [PVZ07]). 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 5.43, the matrices  $P(1), P(2), P(3)$  and  $P(4)$  take the form (5.16) 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 5.46 one should have  $P(1)_{23} + P(2)_{13} + P(3)_{12} = 3 \times 1 - 3 = 0$ , so we reach a contradiction.

It can also be shown that  $\vartheta\text{-rank}(H_8) \geq 2$ , the arguments are similar but technical, so we omit them. So, we have  $\vartheta\text{-rank}(G_8) = \vartheta\text{-rank}(H_8) = 2$ . In

fact,  $G_8$  and  $H_8$  are the only critical graphs on 8 nodes with  $\vartheta$ -rank = 2. To see this, one can use the list of critical graphs on 8 nodes from [Sma15] and verify that all of them have  $\vartheta$ -rank at most 1 except  $G_8$  and  $H_8$ . Note also that, as observed in [PVZ07], any graph with at most 7 nodes has  $\vartheta$ -rank at most 1.

**5.4.2. Adding isolated nodes to graphs with  $\vartheta$ -rank 1.** As we saw in Section 5.2, it is crucial to understand the role of isolated nodes for the  $\vartheta$ -rank of a graph (recall Proposition 5.17). Here, we investigate how many isolated nodes can be added to a graph  $H$  with  $\vartheta$ -rank 1 (and satisfying certain properties) without increasing its  $\vartheta$ -rank. As an application, we show that adding an isolated node to some  $\vartheta$ -rank 1 graphs may produce a graph with  $\vartheta$ -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,  $\alpha$  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  $\vartheta$ -rank 0 for any  $\alpha$ . 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  $H$ .

**Upper bound on the number of isolated nodes.** First, we investigate some necessary conditions about the parameters  $\alpha$  and  $k$  that must hold if  $\vartheta$ -rank( $G$ ) = 1.

**Theorem 5.48.** *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  $\vartheta$ -rank( $G$ ) = 1. Then, we have*

$$\alpha \leq \frac{k(k+3)}{k-1} = k + 4 + \frac{4}{k-1}. \quad (5.17)$$

The rest of the section is devoted to the proof of Theorem 5.48. Throughout we assume that  $G$  and  $H$  are as defined in Theorem 5.48, so that  $M_G = \alpha(A_G + I) - J \in \mathcal{K}_n^{(1)}$ . We will use the following result of Dobre and Vera [DV15], which shows the existence of a  $\mathcal{K}^{(1)}$ -certificate for  $M_G$ , which inherits some symmetry properties of  $M_G$ .

**Proposition 5.49** ([DV15]). *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 5.49. In particular, since any permutation  $\sigma \in \text{Sym}(W)$  of the isolated nodes leaves the graph  $G$  invariant, it follows that

$$\begin{aligned} \sigma(P(i)) &= P(\sigma(i)), \text{ i.e., } P(i)_{\sigma(j)\sigma(k)} = P(\sigma(i))_{jk} \\ &\text{for all } \sigma \in \text{Sym}(W) \text{ and } j, k \in V \cup W. \end{aligned} \quad (5.18)$$

We will use this symmetry property repeatedly in the proof. We mention a simple identity that follows as a direct application of Lemma 5.46, which we will also repeatedly use in the rest of the section:

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

(5.19)

if  $\{i, j, k\}$  is contained in a stable set of  $G$  with size  $\alpha(G)$ .

Now we prove some preliminary lemmas and we end with Lemma 5.53, which will directly imply Theorem 5.48. We start with a general property about the structure of the submatrices  $P(i)[W]$  when  $i \in W$  is an isolated node.

**Lemma 5.50.** *There exists a scalar  $b \in \mathbb{R}$  such that the following holds:*

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

PROOF. Let  $i, j, k \in W$  be distinct (isolated) nodes and set  $b := P(i)_{ij}$ . First, we show that  $b$  does not depend on the choice of  $i, j \in W$ . For this, we use the symmetry property from (5.18), 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 5.1, we have  $P(i)_{jj} + 2P(j)_{ij} = \alpha - 3$ , which implies  $P(i)_{jj} = \alpha - 2b - 3$  and thus (ii) holds. Using again (5.18) with  $\sigma = (i, k)$  we obtain  $P(i)_{\sigma(i)\sigma(j)} = P(\sigma(i))_{i,j}$ , and thus  $P(i)_{jk} = P(k)_{ij}$ . Similarly, using  $\sigma = (i, j)$  we get  $P(i)_{\sigma(i)\sigma(k)} = P(\sigma(i))_{ik}$  and thus  $P(i)_{jk} = P(j)_{ik}$ . By using Eq. (5.19) for the nodes  $i, j, k$  we obtain  $P(i)_{jk} = P(j)_{ik} = P(k)_{ij} = -1$ , thus showing (iii).  $\square$

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

**Lemma 5.51.** *Assume the graph  $H_c$  is connected. Then, the matrix  $P(i)$  takes the form*

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

where the blocks are indexed by  $\{i\}, W \setminus \{i\}$  and  $V$ , respectively, and the scalars  $d, \beta, \gamma$  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 5.43(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  $\gamma_i$  and there exists a vector  $b_i \in \mathbb{R}^W$  such that  $P(i)_{jh} = (b_i)_j$  for all  $j \in W, h \in V$ .

Let  $j \neq k \in W \setminus \{i\}$  and  $v \in V$ . By applying Eq. (5.18) 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  $\beta_i$ . We set  $d_i := (b_i)_i$ . Finally, we show that the scalars  $\beta_i, \gamma_i, d_i$  in fact do not depend on the choice of  $i \in W$  and take the values claimed in the lemma.

For this, consider an  $\alpha$ -stable set  $S$  of  $G$ . Then,  $i \in S$  and thus, by Lemma 5.43(i), the columns of  $P(i)$  indexed by  $S$  sum up to zero. Using the identities of Lemma 5.50 combined with the above facts on the remaining entries of  $P(i)$ , we obtain

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

This concludes the proof.  $\square$

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

**Lemma 5.52.** *Assume  $H_c$  is connected. For any  $v \in V$  the submatrix  $P(v)[W \cup \{v\}]$  takes the form*

$$P(v)[W \cup \{v\}] = \left( \begin{array}{c|c} M_b & \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 \\ \hline \frac{\alpha}{2} - \frac{\alpha}{2k} - 1 & \alpha - 1 \end{array} \right), \quad (5.20)$$

where the blocks are indexed by  $W$  and  $\{v\}$ , respectively. Here,  $b \in \mathbb{R}$  is the constant from Lemma 5.50 and the matrix  $M_b$  is indexed by  $V$  and takes the form

$$M_b = \begin{pmatrix} a & c & \cdots & c \\ c & a & \cdots & c \\ \vdots & \vdots & \ddots & \vdots \\ c & c & \cdots & a \end{pmatrix},$$

$$\text{with } a = \alpha - 3 - \frac{2}{k} \left( b(k+1) + 1 - \alpha - b\alpha \right), \quad c = -1 - \frac{2}{k} (b+1). \quad (5.21)$$

PROOF. Consider an isolated node  $i \in W$ . By Lemma 5.1, we have that  $P(v)_{ii} + 2P(i)_{iv} = \alpha - 3$ . 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  $\alpha$ -stable set of  $G$  that contains  $i, j, v$ . Then, by (5.19), 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 5.1, 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.  $\square$

The following lemma gives necessary and sufficient conditions for the matrix in Equation (5.20) to be positive semidefinite. In particular, the part (ii) of the lemma shows Theorem 5.48.

**Lemma 5.53.** *The matrix in Eq. (5.20) 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 (5.20) with respect to its  $(v, v)$ -entry, we obtain that  $P(v)[W \cup \{v\}] \succeq 0$  if and only if

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

This happens if and only 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

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

and the constant coefficient is

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

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

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

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

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

$$\iff 4k^3\alpha - 4k^3 \geq \alpha^3(k-1)^2 - \alpha^2k(k-1)^2 - 4\alpha^2k(k-1) + 4\alpha k^3 - 4k^3$$

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

**Lower bound on the number of isolated nodes.** In Theorem 5.48 we saw that if the subgraph  $H_c$  of critical edges of  $H$  is connected and the graph  $G = H \oplus \overline{K_{\alpha-k}}$ , obtained by adding  $\alpha - k$  isolated nodes to a graph  $H$  with  $\alpha(H) = k$ , has  $\vartheta$ -rank 1, then the parameters  $\alpha$  and  $k$  must satisfy the inequality (5.17). 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  $\vartheta$ -rank 1 property.

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

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

**Lemma 5.54.** *Assume  $\alpha \geq k \geq 2$  satisfy the inequality (5.17), and let  $M := \alpha I_{\alpha-k} - J_{\alpha-k}$ . Then*

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

PROOF. The above matrix corresponds to the matrix in Equation (5.20) with  $b = -1$ , which gives  $a = \alpha - 1$  and  $c = -1$ , so that  $M = M_b = M_{-1}$ . As  $a \geq c$ , using Lemma 5.53, we get the desired result.  $\square$

**Theorem 5.55.** *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  $\alpha, k$  satisfy the inequality (5.17). 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 5.1. Recall Remark 5.2, where we observed that it will suffice to show that the matrices  $P(i)$  belong to the cone  $\mathcal{K}^{(0)}$ . For this, consider the following construction (inspired from [GL07]), where we set  $M := \alpha I_{\alpha-k} - J_{\alpha-k}$ .

- For  $i \in V$ , we set

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

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

- For  $i \in W$ , we set

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

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

First, we show that the matrix  $P(i)$  is positive semidefinite for all  $i \in W$ . Indeed, deleting repeated rows and columns and taking the Schur complement (see Lemma 1.10) with respect to the lower right corner, we get that  $P(i) \succeq 0$  if and only if  $0 \preceq M - \frac{k}{\alpha-k} J_{\alpha-k} = \alpha I_{\alpha-k} - \frac{\alpha}{\alpha-k} J_{\alpha-k}$ , which is indeed true.

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

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

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

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

First, we show that  $Q(i)$  is positive semidefinite. By Lemma 5.54, we know that the submatrix  $Q(i)[W \cup i^\perp]$  is positive semidefinite. We will now show that any column  $C_v$  of  $Q(i)$  indexed by a node  $v \in V \setminus i^\perp$  (in the third block) can be expressed as a linear combination of the columns  $C_u$  indexed by  $u \in W \cup \{i\}$  (in the first two blocks), which directly implies that  $Q(i) \succeq 0$ . Namely, one can show  $C_v = \frac{1}{1-k} (\sum_{j \in W} C_j + C_i) =: C$  by direct inspection of the entries:

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

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

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

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

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

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



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

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

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

To conclude the proof we now need to check that the linear constraints (ii)-(iv) of Lemma 5.1 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  $P(u)_{vv} + 2P(v)_{uv} = \frac{\alpha^2}{k} - 1 + 2(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}) = \alpha - 3$ .

**Inequality (iv):** We check

$$P(u)_{vw} + P(v)_{uw} + P(w)_{uv} \leq (M_G)_{uv} + (M_G)_{vw} + (M_G)_{vw}$$

for distinct  $u, v, w \in I \cup V$ :

- for  $i, j, k \in I$  we have  $P(i)_{jk} + P(j)_{ik} + P(k)_{ij} = -3$ ,
- for  $i, j \in I, v \in V$  we have  $P(i)_{jv} + P(j)_{iv} + P(v)_{ij} = -3$ ,
- for  $i \in I, u, v \in V$  we have
  - if  $\{u, v\} \notin E$  then

$$P(i)_{uv} + P(u)_{iv} + P(v)_{iu} = \frac{\alpha - k}{k} - 2(\frac{\alpha}{2k} + 1) = -3,$$

– if  $\{u, v\} \in E$  then

$$P(i)_{uv} + P(u)_{iv} + P(v)_{iu} = \frac{\alpha - k}{k} + 2(\frac{\alpha}{2} - \frac{\alpha}{2k} - 1) = \alpha - 3,$$

- for  $u, v, w \in V$  we have
  - if  $\{u, v\}, \{v, w\}, \{u, w\} \in E$  then

$$P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = 3(\alpha - 1),$$

– if  $\{u, v\}, \{u, w\} \in E, \{v, w\} \notin E$  then

$$P(u)_{vw} + P(v)_{uw} + P(w)_{uv} = \alpha - 1 + 2(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}) = 2\alpha - 3 - \frac{\alpha^2}{2k} \leq 2\alpha - 3,$$

$$\begin{aligned}
 & - \text{if } \{u, v\} \in E, \{u, w\}, \{v, w\} \notin E \text{ then} \\
 P(u)_{vw} + P(v)_{uw} + P(w)_{uv} &= 2\left(\frac{\alpha}{2} - 1 - \frac{\alpha^2}{2k}\right) + \frac{\alpha^2}{k} - 1 = \alpha - 3, \\
 & - \text{if } \{u, v\}, \{u, w\}, \{v, w\} \notin E \text{ then} \\
 P(u)_{vw} + P(v)_{uw} + P(w)_{uv} &= -3.
 \end{aligned}$$

This completes the proof. □

We now give some examples of graphs for which the conditions of Theorems 5.48 and 5.55 hold, so that we are able to compute the exact number of isolated nodes that can be added with the resulting graph still having  $\vartheta$ -rank equal to 1.

**Corollary 5.56.** *For any integer  $n \geq 2$  the following holds:*

- (i):  $\vartheta$ -rank( $C_{2n+1} \oplus \overline{K_m}$ ) = 1 if and only if  $m \leq 4 + \frac{4}{n-1}$ .
- (ii):  $\vartheta$ -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 5.21,  $H$  satisfies the property:  $\vartheta$ -rank( $H \setminus i^\perp$ ) = 0 for all  $i \in V$ , and thus the assumption of Theorem 5.55 holds. For  $H = C_{2n+1}$ , the inequality (5.17) reads  $m \leq 4 + \frac{4}{n-1}$  and, for  $H = \overline{C_{2n+1}}$ , it reads  $m \leq 8$ . So the ‘if part’ in both (i), (ii) follows as a direct application of Theorem 5.55.

The ‘only if’ part in both (i), (ii) follows as a direct application of Theorem 5.48, since the graph  $C_{2n+1}$  is critical while the subgraph of critical edges of  $\overline{C_{2n+1}}$  is a connected graph. □

**Corollary 5.57.** *Assume  $H$  is a graph with  $\overline{\chi}(H) > \alpha(H) = 2$ . Then,  $\vartheta$ -rank( $H \oplus \overline{K_m}$ ) = 1 if and only if  $m \leq 8$ .*

PROOF. The ‘if’ part follows directly from Theorem 5.55. Now we prove that  $\vartheta$ -rank( $H \oplus \overline{K_m}$ )  $\geq 2$  for  $m \geq 9$ . Since  $H$  is not perfect it contains the graph  $H_0 = C_5$  or  $H_0 = \overline{C_{2n+1}}$  ( $n \geq 2$ ) as an induced subgraph. Hence,  $H_0 \oplus \overline{K_m}$  is an induced subgraph of  $H \oplus \overline{K_m}$  with the same stability number. Then, by Lemma 5.8,  $\vartheta$ -rank( $H \oplus \overline{K_m}$ )  $\geq \vartheta$ -rank( $H_0 \oplus \overline{K_m}$ )  $\geq 2$ , where the last inequality follows from Corollary 5.56. □

**Corollary 5.58.** *Consider a graph  $H$  and a connected component  $H_0$  of  $H$ . Assume  $\alpha(H_0) \geq 2$  and the subgraph  $(H_0)_c$  of critical edges of  $H_0$  is connected. Then, the following holds:*

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

PROOF. By Corollary 5.27, we know  $\vartheta$ -rank( $H_0$ )  $\geq 1$ . Pick a stable set  $W \subseteq V(H \setminus H_0)$  such that  $\alpha(H_0 \oplus W) = \alpha(H)$ , i.e.,  $|W| = \alpha(H) - \alpha(H_0)$ . Then,  $H_0 \oplus W$  is an induced subgraph of  $H$  with the same stability number

as  $H$ . Then, by Lemma 5.8,  $\vartheta\text{-rank}(H_0 \oplus W \oplus \overline{K_s}) \leq \vartheta\text{-rank}(H \oplus \overline{K_s})$  for any  $s \geq 0$ . By applying Corollary 5.57 to the graph  $H_0$ , we obtain that  $\vartheta\text{-rank}(H_0 \oplus W \oplus \overline{K_s}) \geq 2$  if  $s + |W| \geq 9$ . From these facts, (i) and (ii) now follow easily.  $\square$

### 5.5. Bounds $\nu^{(r)}$ and some extreme graph classes

We finish this chapter by analyzing the bounds  $\nu^{(r)}(G)$  introduced by Peña Vera and Zuluaga [PVZ07] as the analog of the bounds  $\vartheta^{(r)}$ , but using the cones  $\mathcal{Q}_n^{(r)}$  instead of the cones  $\mathcal{K}_n^{(r)}$ . Thus, for a graph  $G = (V = [n], E)$ , the bounds  $\nu^{(r)}(G)$  are defined as

$$\nu^{(r)}(G) := \min \left\{ t : t(A_G + I) - J \in \mathcal{Q}_n^{(r)} \right\}. \quad (5.22)$$

Clearly, we have  $\alpha(G) \leq \vartheta^{(r)}(G) \leq \nu^{(r)}(G) \leq \zeta^{(r)}(G)$  as  $\mathcal{C}_n^{(r)} \subseteq \mathcal{Q}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}$ . Thus,  $\nu^{(r)}(G)$  converges asymptotically to  $\alpha(G)$  as  $r \rightarrow \infty$ . It was shown that Conjecture 3.7 holds for graphs with  $\alpha(G) \leq 8$ , i.e.,  $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$  for graphs with  $\alpha(G) \leq 8$ . It was observed in [GL07] (see also [PVZ07]) that the proof of this result extends to the bounds  $\nu^{(r)}$ , that is,  $\nu^{(\alpha(G)-1)}(G) = \alpha(G)$  for graphs with  $\alpha(G) \leq 8$ , i.e.,  $M_G \in \mathcal{Q}_n^{(\alpha(G)-1)}$  for graphs with  $\alpha(G) \leq 8$ . We define the  $\nu$ -rank as the analog of the  $\vartheta$ -rank for the bounds  $\nu^{(r)}(G)$ .

**Definition 5.59.** *Let  $G$  be a graph. We define the  $\nu$ -rank of  $G$  as*

$$\nu\text{-rank}(G) = \min\{r \in \mathbb{N} : \nu^{(r)}(G) = \alpha(G)\}.$$

*We set  $\nu\text{-rank}(G) = \infty$  if such  $r$  does not exist.*

It is not known whether  $\nu\text{-rank}(G)$  is finite or not for every graph  $G$ . It was pointed out in [DV15] that few graphs are known to have large  $\nu\text{-rank}(G)$ . In this section, we construct graphs with large  $\nu\text{-rank}$ . Namely, for each integer  $k$  we construct a graph  $L_k$  with  $k + 3\binom{k}{2}$  nodes,  $\alpha(L_k) = k$ , and  $\nu\text{-rank}(L_k) \geq k - 1$  (see Corollary 5.67), thus constructing a class of graphs with unbounded  $\nu\text{-rank}$ . Our approach relies on considering the notion of  $\mathcal{Q}^{(r)}$ -certificate, which is a generalization of the notions of  $\mathcal{K}^{(0)}$ -certificates and  $\mathcal{K}^{(1)}$ -certificates (recall that  $\mathcal{Q}_n^{(0)} = \mathcal{K}_n^{(0)}$  and  $\mathcal{Q}_n^{(1)} = \mathcal{K}_n^{(1)}$ ), and exploiting the structure of the zeros of the form  $x^T M_G x$  to obtain information about the corresponding  $\mathcal{Q}^{(r)}$ -certificates for  $M_G$ . As an application, we give a class of graphs for which  $\nu\text{-rank}(G) \geq \alpha(G) - 1$ , thus showing that, if the result of Conjecture 3.7 holds for the parameters  $\nu^{(r)}(G)$ , then it is tight.

**5.5.1. Certifying membership in the cones  $\mathcal{Q}_n^{(r)}$ .** We recall the definition of the cones  $\mathcal{Q}_n^{(r)}$  in relation (1.25): A symmetric matrix  $M \in \mathcal{S}^n$

belongs to  $\mathcal{Q}_n^{(r)}$  if

$$\left(\sum_{i=1}^n x_i\right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n, \\ |\beta|=r, r+2}} \sigma_\beta x^\beta$$

for some  $\sigma_\beta \in \Sigma_{r+2-|\beta|}$ . Observe that we can assume that, in the decomposition, the monomials  $x^\beta$  with  $|\beta| = r + 2$  are square-free. Otherwise, it can be moved to a term of the form  $\sigma_\beta x^\beta$  with  $|\beta| = r$ . The sums of squares  $\sigma_\beta$  corresponding to the monomials  $x^\beta$  with  $|\beta| = r$  have degree 2, and thus take the form  $x^T P(\beta)x$  for some  $n \times n$  positive semidefinite matrix  $P(\beta)$ .

In summary,  $M \in \mathcal{Q}_n^{(r)}$  if, for any  $\beta \in \mathbb{N}^n$  with  $|\beta| = r$ , there exist positive semidefinite matrices  $P(\beta)$ , and, for any  $A \subseteq [n]$  with  $|A| = r + 2$ , there exist nonnegative scalars  $c_A$  such that

$$\left(\sum_{i=1}^n x_i\right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n, \\ |\beta|=r}} x^\beta x^T P(\beta)x + \sum_{\substack{A \subseteq [n] \\ |A|=r+2}} c_A x^A \tag{5.23}$$

We say that  $P(\beta)$  (for  $\beta \in \mathbb{N}^n$ , with  $|\beta| = r + 2$ ) forms a  $\mathcal{Q}^{(r)}$ -certificate for  $M$  if there exist some scalars  $c_A \geq 0$  for  $A \subseteq [n]$  with  $|A| = r + 2$  for which equation (5.23) holds. We now show a result about the structure of the kernel of the matrices in a  $\mathcal{Q}^{(r)}$ -certificate.

**Lemma 5.60.** *Let  $P(\beta)$  (for  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$ ) be a  $\mathcal{Q}^{(r)}$ -certificate for  $M$  and let  $x \in \mathbb{R}_+^n$  such that  $x^T M x = 0$ . Let  $c_A$  (for  $A \subseteq [n]$  with  $|A| = r + 2$ ) be nonnegative scalars such that relation (5.23) holds. Then, for  $\beta \in \mathbb{N}^n$  such that  $\text{Supp}(\beta) \subseteq \text{Supp}(x)$ , we have  $x \in \ker(P(\beta))$ .*

**PROOF.** By evaluating equation (5.23) at  $x$ , the left hand side equals zero, and all terms on the right hand side are nonnegative. Hence, every term on the right hand side should vanish. In particular, if  $\text{Supp}(\beta) \subseteq \text{Supp}(x)$ , then  $x^\beta > 0$ . This implies that  $x^T P(\beta)x = 0$ . Hence,  $P(\beta)x = 0$  as  $P(\beta) \succeq 0$ .  $\square$

**5.5.2. Graph matrices and  $\nu$ -rank.** In this section, we specialize the result of Lemma 5.60 to the case of graph matrices  $M_G$ . We first show the following preliminary result.

**Lemma 5.61.** *Let  $G = ([n], E)$  be a graph and let  $r \geq 0$ . Assume  $\nu\text{-rank}(G) \leq r$ , i.e.,  $M_G \in \mathcal{Q}_n^{(r)}$ . Let  $P(\beta)$  (for  $\beta \in \mathbb{N}^n$  with  $|\beta| = r + 2$ ) be a  $\mathcal{Q}^{(r)}$ -certificate for  $M_G$ . Let  $C_1, C_2, \dots, C_n$  be the columns of the matrix  $P(\beta)$  for a fixed  $\beta \in \mathbb{N}^n$ . Assume  $S := \text{Supp}(\beta)$  is stable and  $\alpha(G \setminus S^\perp) = \alpha(G) - |S|$ . Then, for any critical edge  $\{i, j\}$  of  $G \setminus S^\perp$ , we have  $C_i = C_j$ .*

**PROOF.** Since  $\{i, j\}$  is critical in  $G \setminus S^\perp$ , then there exists  $I \subseteq V$  such that  $I \cup \{i\}$  and  $I \cup \{j\}$  are stable of size  $\alpha(G \setminus S^\perp) = \alpha(G) - |S|$  in  $G \setminus S^\perp$ . Then,  $S \cup I \cup \{i\}$  and  $S \cup I \cup \{j\}$  are stable of size  $\alpha(G)$  in  $G$ . Let  $x = \chi^{S \cup I \cup \{i\}}$  and

$y = \chi^{S \cup I \cup \{j\}}$  be the indicator vectors of  $S \cup I \cup \{i\}$  and  $S \cup I \cup \{j\}$ . Then,  $x^T M_G x = 0$  and  $y^T M_G y = 0$ , in view of relation (5.8) and Theorem 5.7. Then, by Lemma 5.60,  $x, y \in \ker(P(\beta))$ , so that  $x - y = \chi^{\{i\}} - \chi^{\{j\}} \in \ker(P(\beta))$ . This implies  $C_i = C_j$ .  $\square$

Now, we state the main result of this section. For this, we recall that the graph  $G_c = (V, E_c)$  of critical edges of  $G = (V, E)$  is obtained by deleting the non-critical edges of  $G$  while keeping the same vertex set.

**Theorem 5.62.** *Let  $G = ([n], E)$  be a graph and let  $S$  be a stable set of  $G$  such that  $\alpha(G \setminus S^\perp) = \alpha(G) - |S|$ . Assume that for any subset  $S' \subseteq S$  with  $|S'| = |S| - 2$  we have that the graph  $(G \setminus S'^\perp)_c$  is connected. Then, we have  $\nu\text{-rank}(G) \geq |S| - 1$ .*

PROOF. We show that  $M_G \notin \mathcal{Q}_n^{|S|-2}$  by contradiction. We set  $|S| - 2 = r$ . Assume  $M_G \in \mathcal{Q}_n^{(r)}$ , and let  $P(\beta)$  (for  $\beta \in \mathbb{N}^n$  with  $|\beta| = r$ ) be a  $\mathcal{Q}^{(r)}$ -certificate for  $M_G$ . Then, there exist scalars  $c_A \geq 0$  (for  $A \subseteq [n]$ , with  $|A| = r + 2$ ) such that the following equation holds:

$$\left( \sum_{i=1}^n x_i \right)^r x^T M_G x = \sum_{\substack{\beta \in \mathbb{N}^n, \\ |\beta|=r}} x^\beta x^T P(\beta) x + \sum_{\substack{S \subseteq [n] \\ |A|=r+2}} c_A x^A. \quad (5.24)$$

We will reach a contradiction by comparing the coefficient of  $x^S (= \prod_{i \in S} x_i)$  in Equation (5.24) at both sides. On the left hand side, the coefficient is  $-(r+2)(r+1) < 0$ . On the right hand side, the coefficient of  $x^S$  is

$$\sum_{\substack{S' \subseteq V \\ S' \cup \{i, j\} = S}} 2P(S')_{ij} + c_S.$$

We will show that all terms in the first summation are nonnegative. Let  $S' \subseteq S$ , with  $S' \cup \{i, j\} = S$ . Observe that  $\alpha(G \setminus S'^\perp) = \alpha(G) - |S'|$ , because  $\alpha(G \setminus S^\perp) = \alpha(G) - |S|$  and  $S' \subseteq S$ . By Lemma 5.61, if  $\{v_1, v_2\}$  is a critical edge of  $G \setminus S'^\perp$ , then the columns of  $P(S')$  indexed by  $v_1$  and  $v_2$  are equal. Using that  $(G \setminus S'^\perp)_c$  is connected, we obtain that all columns of  $P(S')$  indexed by vertices of  $G \setminus S^\perp$  are identical. In particular, the columns indexed by  $i$  and  $j$  are equal. This implies that  $P(S')_{ij} = P(S')_{ii}$ , which is nonnegative as  $P(S') \succeq 0$ . Using that  $c_S \geq 0$ , we reach a contradiction as the coefficient of  $x^S$  on the right hand side is positive while on the left hand side it is negative.  $\square$

**5.5.3. Graph classes with large  $\nu$ -rank.** In this section, we show examples of graphs with large  $\nu$ -rank. We first recall the two graph classes  $(G_k)_{k \in \mathbb{N}}$  and  $(H_k)_{k \in \mathbb{N}}$  introduced in [PVZ07] and [DV15]. It was conjectured (with another language) that  $\nu\text{-rank}(L_k) \rightarrow \infty$  and  $\vartheta\text{-rank}(G_k) \rightarrow \infty$  as  $k \rightarrow \infty$ .

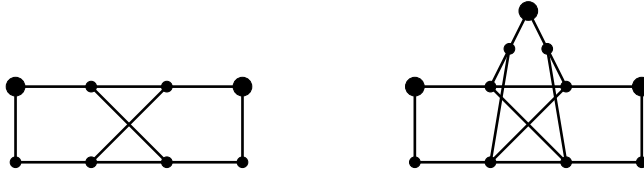


FIGURE 5.9. Graphs  $H_8$  and  $H_{11}$ .

**Graphs  $H_k$ .** Peña, Vera and Zuluaga [PVZ07] proposed the graphs  $H_8, H_{11}, H_{14}$  and  $H_{17}$  shown in Figures 5.9 and 5.10. We have that  $\alpha(H_8) = 3, \alpha(H_{11}) = 4, \alpha(H_{14}) = 5$  and  $\alpha(H_{17}) = 6$ .



FIGURE 5.10. Graphs  $H_{14}$  and  $H_{17}$ .

It was shown numerically (see [PVZ07] and [DV15]) that  $\nu\text{-rank}(G) > \alpha(G) - 2$  for  $G = H_8, H_{11}$  and  $H_{14}$ , and it was conjectured the same result for  $H_{17}$ . We give an analytical proof of a slightly weaker version of the property just mentioned, as a direct application of Theorem 5.62.

**Corollary 5.63.** *For  $i = 8, 11, 14, 17$ , we have  $\nu\text{-rank}(H_i) > \alpha(H_i) - 3$ .*

PROOF. We apply Theorem 5.62. For each graph  $H_k$  with  $k = 8, 11, 14, 17$ , we take  $S$  as the set of vertices highlighted (big vertices) in each graph. For each case  $k = 8, 11, 14, 17$ , we have that  $H_k \setminus S^\perp$  is the complete graph  $K_2$ , thus  $\alpha(H \setminus S^\perp) = 1 = \alpha(H_k) - |S|$ . To check the next condition, we first observe that the graph  $H_8$  is critical. Now, note that in all cases, for any  $S' \subseteq S$  with  $|S'| = |S| - 2$ , the graph  $G \setminus S'^\perp$  is isomorphic to  $H_8$ , and thus  $(G \setminus S'^\perp)_c$  is connected. This concludes the proof.  $\square$

**Graphs  $G_k$ .** Dobre and Vera [DV15] defined the following class of graphs  $G_k$  for  $k \geq 1$ .

**Definition 5.64.** *Let  $K_{k+1, k+1}$  be the complete bipartite graph with bipartition  $(U, V)$  with  $U = \{u_0, u_1, \dots, u_k\}$  and  $V = \{v_0, v_1, \dots, v_k\}$ . The graph  $G_k$  is obtained by adding a node  $w_i$  in-between the edge  $\{u_i, v_i\}$  for all  $i = 1, 2, \dots, k$ ; that, is deleting the edge  $\{u_i, v_i\}$  and adding the edges  $\{u_i, w_i\}$  and  $\{v_i, w_i\}$ . We show  $G_2$  and  $G_k$  in Figure 5.11.*

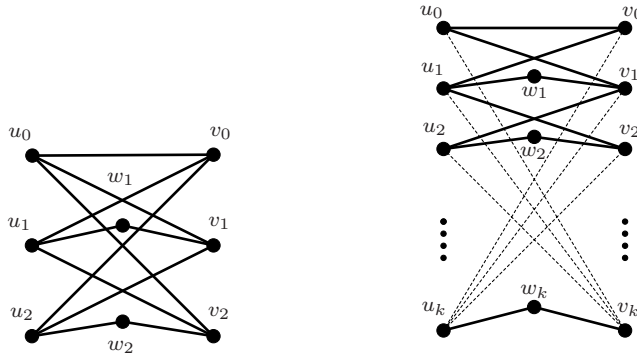


FIGURE 5.11. Graphs  $G_2$  and  $G_k$

It was observed in [DV15] that  $\alpha(G_k) = k + 1$ , and it was conjectured that  $\nu\text{-rank}(G_k) > k - 1$ . We show that  $\nu\text{-rank}(G_k) > k - 2$  as an application of Theorem 5.62.

**Corollary 5.65.** *Let  $G_k$  be the graph defined above. Then, we have  $\nu\text{-rank}(G_k) > k - 2$ , i.e.,  $\nu^{(k-2)}(G_k) > \alpha(G_k)$ .*

PROOF. We set  $S = \{w_1, w_2, \dots, w_k\}$ , then  $\alpha(G \setminus S^\perp) = 1$ . For any subset  $S' \subseteq S$  with  $|S'| = k - 2$ , the graph  $G \setminus S'^\perp$  is isomorphic to  $G_2$ . We observe that the edges  $\{u_0, v_0\}$ ,  $\{u_1, w_1\}$ ,  $\{w_1, v_1\}$ ,  $\{u_2, w_2\}$ ,  $\{w_2, v_2\}$ ,  $\{u_0, v_2\}$  and  $\{v_2, u_0\}$  are critical in  $G_2$ , therefore  $(G_2)_c$  is connected. Hence, by Theorem 5.62, we obtain that  $\nu\text{-rank}(G_k) \geq k - 1$ .  $\square$

**New class of graphs  $L_k$ .** We define the following class of graphs  $L_k$ . We start with a set of vertices  $S_k = \{s_1, \dots, s_k\}$ . For any pair of distinct nodes  $s_i, s_j$  of  $S$  we construct three extra nodes  $a_{ij}, b_{ij}, c_{ij}$  and we construct the edges  $\{s_i, a_{ij}\}, \{a_{ij}, b_{ij}\}, \{b_{ij}, s_j\}, \{s_j, c_{ij}\}, \{c_{ij}, s_i\}$  so that the nodes  $s_i, a_{ij}, b_{ij}, s_j, c_{ij}$  form a 5-cycle. Finally, we construct a bipartite graph  $K_{3,3}$  between the nodes  $\{a_{ij}, b_{ij}, c_{ij}\}$  and  $\{a_{lm}, b_{lm}, c_{lm}\}$  if  $\{i, j\} \neq \{l, m\}$ . So,  $L_k$  has  $k + 3\binom{k}{2}$  nodes.

**Lemma 5.66.** *Let  $L_k$  be as above, then  $\alpha(L_k) = k$ .*

PROOF. Note that  $S_k$  is stable of size  $k$  in  $L_k$ . We now show that there is no stable set of size  $k + 1$  in  $L_k$ . Let  $A \subseteq V$  be a stable set in  $L_k$ . By construction,  $A$  could contain elements of type  $a_{ij}, b_{ij}$  and  $c_{ij}$  from just one pair  $(i, j)$ . Assume that  $(1, 2)$  is such pair, so that  $\{a_{ij}, b_{ij}, c_{ij}\} \cap A = \emptyset$  if  $(i, j) \neq (1, 2)$ . Hence,  $A$  is stable in the graph obtained by deleting all nodes  $a_{ij}, b_{ij}$  and  $c_{ij}$  for  $(i, j) \neq (1, 2)$ , which is isomorphic to the graph  $C_5 \oplus \overline{K_{k-2}}$ . Hence,  $|A| \leq \alpha(C_5 \oplus \overline{K_{k-2}}) = k$ .  $\square$

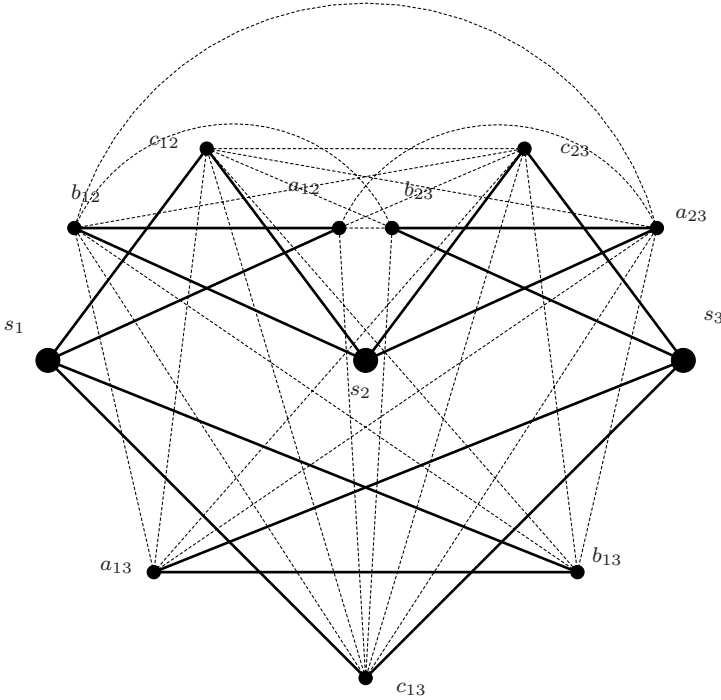


FIGURE 5.12. Graph  $L_3$

**Corollary 5.67.** *For any  $k \geq 2$ , we have  $\nu\text{-rank}(L_k) > \alpha(L_k) - 2$ , i.e.,  $\nu^{(\alpha(L_k)-2)}(L_k) > \alpha(L_k)$ .*

PROOF. We check that the set  $S_k$  satisfies the conditions of Theorem 5.62. The graph  $G \setminus S_k^\perp$  is the empty graph, so we have  $0 = \alpha(L_k \setminus S_k^\perp) = \alpha(L_k) - |S_k|$ . Now, for any subset  $S' \subseteq S_k$  with  $|S'| = k - 2$ , the graph  $L_k \setminus S'^\perp$  is isomorphic to  $C_5$ , which is critical and connected. Then, by Theorem 5.62, we have  $\nu\text{-rank}(L_k) \geq |S_k| - 1 = \alpha(L_k) - 1$ .  $\square$

**Discussion and open problems about the parameter  $\nu^{(r)}(G)$ .** It remains open whether all graph matrices  $M_G$  belong to some cone  $\mathcal{Q}_n^{(r)}$ . In other words, whether the hierarchy  $\nu^{(r)}(G)$  has finite convergence to  $\alpha(G)$ . The result of Corollary 5.67 shows that, if the analog of Conjecture 3.7 holds for the parameter  $\nu^{(r)}(G)$  (i.e.,  $\nu\text{-rank}(G) \leq \alpha(G) - 1$ ), then the result is tight. Recall that this result holds for any graph  $G$  with  $\alpha(G) \leq 8$  (see [GL07]). Therefore, for  $k = 2, \dots, 8$ , we have  $\nu\text{-rank}(L_k) = \alpha(L_k) - 1 = k - 1$ , i.e.,  $M_{L_k} \in \mathcal{Q}^{(k-1)} \setminus \mathcal{Q}^{(k-2)}$ . It remains open whether this holds for all  $k \in \mathbb{N}$ .



## CHAPTER 6

### Test states and membership in quadratic modules

*This chapter is based on my joint work [SV23] with Markus Schweighofer.*

In this chapter, we prove two main results already announced in Chapters 2 and 3, namely, Theorems 2.2 and 3.8. Recall that these two results claim, respectively, that

$$\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}, \quad (6.1)$$

and that the hierarchy  $\vartheta^{(r)}(G)$  has always finite convergence, that is, we have

$$M_G \in \bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \text{ for every graph } G = ([n], E). \quad (6.2)$$

Recall that, in Theorem 2.3 in Chapter 2, we show that to prove Theorem 2.2 (i.e., that relation (6.1) holds) it suffices to show that every positive diagonal scaling of the Horn matrix belongs to some cone  $\mathcal{K}_5^{(r)}$ . We show this result.

**Theorem 6.1.** *Let  $D = \text{Diag}(d_1, \dots, d_5)$  with  $d_i > 0$  for  $i \in [5]$ . Then,*

$$DHD \in \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}.$$

Also, in Proposition 5.19 in Chapter 5, we showed that the hierarchy  $\vartheta^{(r)}(G)$  has finite convergence to  $\alpha(G)$  (i.e.,  $\vartheta\text{-rank}(G) < \infty$  for all  $G$ ) if and only if the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  is preserved after adding isolated nodes (i.e.,  $\vartheta\text{-rank}(G) < \infty$  implies  $\vartheta\text{-rank}(G \oplus i_0) < \infty$ ). We show that this last claim holds, and thus we obtain the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  for every graph  $G$ .

**Theorem 6.2.** *Let  $G = (V = [n], E)$  be a graph such that  $\vartheta\text{-rank}(G) < \infty$ . Then,  $\vartheta\text{-rank}(G \oplus i_0) < \infty$ .*

Now, we briefly summarize the strategy of the proof of Theorems 6.1 and 6.2, for which we will use a similar idea in both cases.

**Reformulations of the Theorems.** First, using relation (2.1) in Chapter 2 (see also [dKP02]), we have that, for all  $n \geq 1$ ,

$$\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} = \bigcup_{r \geq 0} \text{LAS}_{\mathbb{S}^{n-1}}^{(r)}. \quad (6.3)$$

Recall that

$$M \in \bigcup_{r \geq 0} \text{LAS}_{\mathbb{S}^{n-1}}^{(r)} \iff (x^{\circ 2})^T M x^{\circ 2} \in \Sigma + I\left(\sum_{i=1}^n x_i^2 - 1\right).$$

Then, we can reformulate Theorems 6.1 and 6.2 as follows.

**Theorem 6.3.** *Let  $D = \text{Diag}(d_1, \dots, d_5)$  with  $d_i > 0$  for  $i \in [5]$ . Then,*

$$(x^{\circ 2})^T D H D x^{\circ 2} \in \Sigma + I\left(\sum_{i=1}^5 x_i^2 - 1\right). \quad (6.4)$$

**Theorem 6.4.** *Let  $G = (V = [n], E)$  be a graph such that  $\vartheta\text{-rank}(G) < \infty$  (i.e.,  $(\sum_{i=1}^n x_i^2)^r f_G \in \Sigma$  for some  $r \in \mathbb{N}$ ). Then, we have*

$$f_{G \oplus i_0} \in \Sigma + I\left(x_{i_0}^2 + \sum_{i=1}^n x_i^2 - 1\right). \quad (6.5)$$

Recall that  $f_G = (x^\circ)^T M_G x^{\circ 2}$ . So, in both cases, we need to show the membership of a (quartic) form in some quadratic module.

**Membership in quadratic modules.** Given a polynomial  $f$  and sets of polynomials  $\mathbf{g} = \{g_1, \dots, g_m\}$  and  $\mathbf{h} = \{h_1, \dots, h_l\}$ , a fundamental question in real algebraic geometry is to decide whether  $f \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h})$ . Recall that the sets  $\mathcal{M}(\mathbf{g})$  and  $I(\mathbf{h})$  are defined as

$$\mathcal{M}(\mathbf{g}) := \left\{ \sum_{i=0}^m \sigma_i g_i : \sigma_i \in \Sigma \text{ for } i = 0, 1, \dots, m, \text{ and } g_0 := 1 \right\},$$

and

$$I(\mathbf{h}) := \left\{ \sum_{i=1}^l p_i h_i : p_i \in \mathbb{R}[x] \text{ for } i \in [l] \right\}.$$

Observe that for showing that relations (6.4) and (6.5) hold we shall prove that the polynomials  $(x^{\circ 2})^T D H D x^{\circ 2}$  and  $f_{G \oplus i_0}$  belong to a particular quadratic module  $\mathcal{M}(\mathbf{g}) + I(\mathbf{h})$ . Clearly, if  $f \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h})$ , then  $f \geq 0$  on the semialgebraic set

$$K = \left\{ x \in \mathbb{R}^n : g_i(x) \geq 0 \text{ for } i \in [m], h_j(x) = 0 \text{ for } j \in [l] \right\}.$$

Then, a necessary condition for a polynomial  $f$  for belonging to  $\mathcal{M}(\mathbf{g}) + I(\mathbf{h})$  is to be nonnegative on  $K$ . On the positive side, if  $f > 0$  on  $K$  and the polynomial sets  $\mathbf{g}$  and  $\mathbf{h}$  satisfy the Archimedean condition (1.15), then  $f$

belongs to  $\mathcal{M}(\mathbf{g}) + I(\mathbf{h})$  by Putinar's theorem (see Theorem 1.9). Also, if  $f \geq 0$  on  $K$ ,  $f$  has finitely many zeros on  $K$ , and they satisfy some technical conditions, then  $f \in \mathcal{M}(\mathbf{g}) + I(\mathbf{h})$  by Nie's theorem (see Theorem 1.13). The point, however, is that the polynomials  $(x^{\circ 2})^T DHDx^{\circ 2}$  and  $f_{G \oplus i_0}$  have infinitely many minimizers on their corresponding semialgebraic sets. Hence, the last two results cannot be applied.

In this chapter, we develop a tool for testing membership in quadratic modules (Theorem 6.22). This result, which itself is based on a result shown in [BSS12], permits to certify that a polynomial belongs to a quadratic module even when the polynomial has infinitely many zeros on its associated semialgebraic set. As a main application, we prove Theorems 6.3 and 6.4.

## 6.1. Preliminaries

**Membership in cones and pure states.** Let  $V$  be a vector space over  $\mathbb{R}$ , and let  $C \subseteq V$  be a convex cone, i.e.,  $0 \in C$ ,  $C + C \subseteq C$  and  $\mathbb{R}_+ C \subseteq C$ . In this section, we recap a useful tool for showing that a vector  $v \in V$  belongs to the cone  $C$ . The definition and results of this preliminary section are based on [BSS12] and [Schw22]. A very good and detailed exposition is given in [Schw22, Chapter 7]. We will use this machinery repeatedly. We introduce the following notions.

**Definition 6.5.** *Let  $C$  be a convex cone in the  $\mathbb{R}$ -vector space  $V$  and  $u \in V$ . Then,  $u$  is called a unit of  $C$  (in  $V$ ) if, for every  $x \in V$ , there is some  $N \in \mathbb{N}$  such that  $Nu + x \in C$ .*

**Definition 6.6.** *Let  $V$  be a vector space on  $\mathbb{R}$ ,  $C \subseteq V$  a convex cone, and  $u \in V$ . A state of  $(V, C, u)$  is a linear function  $\varphi : V \rightarrow \mathbb{R}$  satisfying  $\varphi(C) \subseteq \mathbb{R}_+$  and  $\varphi(u) = 1$ . The (convex) set of all states of  $(V, C, u)$  is denoted by  $S(V, C, u)$ . We say that  $\varphi \in S(V, C, u)$  is a pure state if it is an extreme point of  $S(V, C, u)$ .*

Clearly, if  $x \in C$ , the  $\varphi(x) \geq 0$  for all pure states of  $S(V, C, u)$ . The following result shows that the reverse implication holds under a "strict positivity" assumption.

**Theorem 6.7** ([EHS80], see also Corollary 7.3.20 in [Schw22]). *Suppose  $u$  is a unit for the cone  $C$  in the vector space  $V$  over  $\mathbb{R}$  and let  $x \in V$ . If  $\varphi(x) > 0$  for all pure states  $\varphi$  of  $S(V, C, u)$ , then there exists  $\varepsilon > 0$  such that  $x - \varepsilon u \in C$ . In particular,  $x \in C$ .*

**Preorders and dichotomy theorem.** In this section, we recall a result from [BSS12] (see also [Schw22]) in which the pure states of a very special setting are characterized. This result will be used in Section 6.2 for giving a criterion for testing membership in quadratic modules.

**Definition 6.8.** *Let  $A$  be a commutative ring. The subset  $T \subseteq A$  is called a preorder of  $A$  if  $A^2 := \{a^2 : a \in A\} \subseteq T$ ,  $T + T \subseteq T$  and  $TT \subseteq T$ .*

Given a preorder  $T$  of  $A$ , we say that  $M \subseteq A$  is a  $T$ -module of  $A$  if  $0 \in M$ ,  $M + M \subseteq M$ , and  $TM \subseteq M$ .

Observe that, in the situation of the above definition, we can think of an ideal  $I$  of  $A$  as a vector space and of  $M$  as a cone in  $I$ . So, we can consider the state space  $S(I, M, u)$  for a unit  $u$  for  $M$  in  $I$ . The following result characterizes the pure states in this situation.

**Theorem 6.9** (Dichotomy theorem [BSS12]). *Let  $A$  be a commutative ring with  $\mathbb{R} \subset A$ . Suppose that  $I$  is an ideal of  $A$ ,  $T$  is a preorder of  $A$ ,  $M \subseteq I$  is a  $T$ -module of  $A$ ,  $u$  is a unit for  $M$  in  $I$ , and  $\varphi$  is a pure state of  $(I, M, u)$ . Then, exactly one of the following two assertions holds.*

- (i)  $\varphi$  is the restriction of a scaled ring homomorphism: There exists a ring homomorphism  $\Phi : A \rightarrow \mathbb{R}$  such that  $\Phi(u) \neq 0$  and  $\varphi = \frac{1}{\Phi(u)}\Phi|_I$ .
- (ii) There exists a ring homomorphism  $\Phi : A \rightarrow \mathbb{R}$  with  $\Phi|_I = 0$  such that

$$\varphi(ab) = \Phi(a)\varphi(b) \text{ for all } a \in A, b \in I.$$

## 6.2. Test states and membership in quadratic modules

In this section we will develop a tool that permits to test membership in quadratic modules of  $\mathbb{R}[x]$ . We first define the notion of quadratic modules.

**Definition 6.10.** *Let  $M \subseteq \mathbb{R}[x]$ . We say that  $M$  is a quadratic module of  $\mathbb{R}[x]$  if  $1 \in M$ ,  $M + M \subseteq M$ , and  $\Sigma M \subseteq M$ . In other words,  $M$  is a quadratic module if  $M$  is a  $\Sigma$ -module of  $\mathbb{R}[x]$  and  $1 \in M$ .*

**Example 6.11.** *Given a set of polynomials  $\mathbf{g}$ , the quadratic module generated by  $\mathbf{g}$  is defined as*

$$\mathcal{M}(\mathbf{g}) = \left\{ \sigma + \sum_{i=1}^n g_i \sigma_i : \sigma, \sigma_i \in \Sigma, g_i \in \mathbf{g} \right\}.$$

Observe that, for a finite set  $\mathbf{g}$ ,  $\mathcal{M}(\mathbf{g})$  was already defined in relation (1.10) in Chapter 1.

**Example 6.12.** *Let  $M$  be a quadratic module, and let  $I$  be an ideal in  $\mathbb{R}[x]$ . Then,  $M + I$  is a quadratic module.*

**Definition 6.13.** *We say that the quadratic module  $M$  is Archimedean if for every  $p \in \mathbb{R}[x]$  there exists  $N \in \mathbb{N}$  such that  $N + p \in M$  and  $N - p \in M$ .*

The following result is useful for identifying Archimedean quadratic modules (and shows the equivalence with the definition from relation (1.15) we give in Chapter 1).

**Proposition 6.14** (see, for example [Schw22]). *Let  $M$  be a quadratic module. Then, the following assertions are equivalent:*

- (i)  $M$  is Archimedean.
- (ii) There exists  $N \in \mathbb{N}$  such that  $N - \sum_{i=1}^n x_i^2 \in M$ .

**Example 6.15.** Let  $n \geq 1$  be an integer. Then the set

$$\Sigma + I\left(\sum_{i=1}^n x_i^2 - 1\right)$$

is an Archimedean quadratic module.

**Definition 6.16.** Let  $\mathbf{g} \subseteq \mathbb{R}[x]$  be a set of polynomials. We introduce the nonnegativity set

$$S(\mathbf{g}) := \{x \in \mathbb{R}^n : g(x) \geq 0 \text{ for all } g \in \mathbf{g}\}$$

of  $\mathbf{g}$ . Moreover, for a given polynomial  $f \in \mathbb{R}[x]$ , we denote by

$$Z(f) := \{a \in \mathbb{R}^n \mid f(a) = 0\}$$

its (real) zero set.

**Remark 6.17.** We make the following observations:

- (a) Let  $\mathbf{g}$  be a finite subset of  $\mathbb{R}[x]$ . Then,  $S(\mathbf{g})$  is a basic closed semialgebraic set, i.e., the set of solutions of a finite system of polynomial inequalities (usually denoted by  $K$ ).
- (b) If  $M$  is the quadratic module generated by a subset  $\mathbf{g}$  of  $\mathbb{R}[x]$ , then we have  $S(M) = S(\mathbf{g})$ .
- (c) If  $M$  is a finitely generated quadratic module, then  $S(M)$  is again a basic closed semialgebraic set. This follows from (a) and (b).

Now we define the notion of *test state* that will be useful for stating the main result of this section.

**Definition 6.18.** Let  $V$  be a vector space,  $C \subseteq V$  a convex set,  $u \in V$ , and  $\mathbf{g} \subseteq V$ . We say that  $u$  is  $\mathbf{g}$ -stably contained in  $C$  if, for all  $g \in \mathbf{g}$ , there exists a real  $\varepsilon > 0$  such that  $u + \varepsilon g \in C$  and  $u - \varepsilon g \in C$ .

Note that in the situation of the above definition, if  $\mathbf{g} \neq \emptyset$ , then every element  $\mathbf{g}$ -stably contained in  $C$  is of course contained in  $C$ . We will select  $V$  to be an ideal  $I$  of  $\mathbb{R}[x]$ , and  $C$  to be a quadratic module  $M$  intersected with the ideal  $I$ . In this setting, the following result holds.

**Proposition 6.19.** Let  $\mathbf{g} \subseteq \mathbb{R}[x]$  be a nonempty set, let  $I = I(\mathbf{g})$  be the ideal generated by  $\mathbf{g}$ , let  $M$  be an Archimedean quadratic module of  $\mathbb{R}[x]$ , and let  $u \in \mathbb{R}[x]$  be a polynomial such that  $uM \subseteq M$ . If  $u$  is  $\mathbf{g}$ -stably contained in  $M$ , then  $u$  is  $I$ -stably contained in  $M$ . In particular, if  $u \in I$ , then  $u$  is a unit of the cone  $I \cap M$  in the vector space  $I$ .

**PROOF.** The proof of this result is essentially from [Schw22], where this result is stated in a more general context. We show the proof for completeness.

Consider the set

$$B_u = \{p \in \mathbb{R}[x] : \text{there exists } \varepsilon > 0 \text{ such that } u \pm \varepsilon p \in M\}.$$

We show that  $B_u$  is an ideal of  $\mathbb{R}[x]$ . Clearly,  $p \in B_u$  if and only if  $-p \in B_u$ . Now, if  $u \pm \varepsilon_1 p \in M$  and  $u \pm \varepsilon_2 q \in M$  then  $(\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2})u \pm (p - q) \in M$ . Hence,

$$u \pm \frac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2}}(p - q) \in M.$$

This shows that  $p - q \in B_u$  if  $p, q \in B_u$ .

We finally show that if  $p \in B_u$ , then  $pq \in B_u$  for all  $q \in \mathbb{R}[x]$ . For this, we observe that the following identity holds

$$q = \frac{1}{4}((q+1)^2 - (q-1)^2).$$

Then, it suffices to show that  $pq^2 \in B_u$  for all  $q \in \mathbb{R}[x]$ . Since  $M$  is Archimedean and  $p \in B_u$ , there exists  $N > 0$  such that  $N - q^2 \in M$  and  $Nu \pm p \in M$ . Since  $uM \subseteq M$ , we have  $Nu - uq^2 \in M$ . Since  $\Sigma M \subseteq M$ , we have  $Nuq^2 \pm pq^2 \in M$ . Hence,

$$N^2u \pm pq^2 = (N^2u - Nuq^2) + (Nuq^2 \pm pq^2) \in M + M \subseteq M,$$

as desired.  $\square$

Now we introduce the notion of *test state*.

**Definition 6.20.** Let  $I$  be an ideal and  $M$  be a quadratic module of  $\mathbb{R}[x]$ . Let  $u \in I$  and  $a \in \mathbb{R}^n$ . We call  $\varphi: I \rightarrow \mathbb{R}$  a test state on  $I$  for  $M$  at  $a$  with respect to  $u$  if

- (i)  $\varphi$  is linear,
- (ii)  $\varphi(M \cap I) \subseteq \mathbb{R}_{\geq 0}$ ,
- (iii)  $\varphi(u) = 1$  and  $\varphi(pq) = p(a)\varphi(q)$  for all  $p \in \mathbb{R}[x]$  and  $q \in I$ .

**Remark 6.21.** Let  $\varphi$  be a state as in Definition 6.20. If  $uM \subseteq M$ , then we have that  $a \in Z(g)$  for every  $g \in M \cap (-M)$ . Indeed,  $ug \in M \cap I$ , and  $-ug \in M \cap I$ , so that  $\varphi(gu) = 0$ . Hence,  $\varphi(u)g(a) = g(a) = 0$ .

**Theorem 6.22.** Let  $\mathbf{g} \subseteq \mathbb{R}[x]$  be a nonempty set of polynomials and let  $M$  be an Archimedean quadratic module of  $\mathbb{R}[x]$ . Let  $I = I(\mathbf{g})$  be the ideal generated by  $\mathbf{g}$ . Let  $f \in I$  and  $u \in M \cap I$ . Assume the following assertions hold:

- (i)  $f \geq 0$  on  $S(M)$ .
- (ii)  $Z(f) \cap S(M) \subseteq Z(u) \cap S(M)$ .
- (iii)  $uM \subseteq M$ .
- (iv)  $u$  is  $\mathbf{g}$ -stably contained in  $M$ .
- (v)  $\varphi(f) > 0$  for all test states on  $I$  for  $M$  at a point  $a \in Z(f) \cap S(M)$ .

Then, there is  $\varepsilon > 0$  such that  $f - \varepsilon u \in M$ . In particular,  $f \in M$ .

PROOF. We will apply Theorem 6.7 in the following setting: The vector space is the ideal  $I$ . The cone is  $M \cap I$ . In view of Proposition 6.19, using assumptions (iii) and (iv), we have that  $u$  is a unit of  $I \cap M$  in  $I$ . So, we consider the following *state space*:

$$S := S(I, I \cap M, u) = \{\varphi \mid \varphi: I \rightarrow \mathbb{R} \text{ linear, } \varphi(I \cap M) \subseteq \mathbb{R}_{\geq 0}, \varphi(u) = 1\} \subseteq \mathbb{R}^I.$$

Let  $\varphi$  be a pure state of  $(I, I \cap M, u)$ . We will show that  $\varphi(f) > 0$ . Then, by Theorem 6.7 we can conclude that, for some  $\varepsilon > 0$ , we have  $f - \varepsilon u \in I \cap M \subseteq M$ , as desired. To show  $\varphi(f) > 0$ , we apply Theorem 6.9 in the following setting:  $A$  there is  $\mathbb{R}[x]$  here,  $I$  there is also  $I$  here,  $T$  there is  $\Sigma + u\Sigma$  here,  $M$  there is  $M \cap I$  here, and  $u$  there is also  $u$  here. We show that the assumptions of Theorem 6.9 hold. Clearly,  $\Sigma + u\Sigma$  is a preorder, and using the fact that  $uM \subseteq M$ , we obtain that  $M \cap I$  is a  $(\Sigma + u\Sigma)$ -module. Hence, the assumptions of Theorem 6.9 hold. Then, exactly one of the following two alternatives holds:

- (1)  $\varphi$  is the restriction of a scaled ring homomorphism: There exists a ring homomorphism  $\Phi : \mathbb{R}[x] \rightarrow \mathbb{R}$  such that  $\Phi(u) \neq 0$  and  $\varphi = \frac{1}{\Phi(u)}\Phi|_I$ .
- (2) There exists a ring homomorphism  $\Phi : \mathbb{R}[x] \rightarrow \mathbb{R}$  with  $\Phi|_I = 0$  such that

$$\varphi(pq) = \Phi(p)\varphi(q) \text{ for all } p \in \mathbb{R}[x], q \in I.$$

It is easy to observe that every ring homomorphism  $\Phi : \mathbb{R}[x] \rightarrow \mathbb{R}$  is given by a point evaluation, i.e., there exists  $a \in \mathbb{R}^n$ , such that  $\Phi(p) = p(a)$  for some all  $p \in \mathbb{R}[x]$ . Therefore,  $\varphi$  is determined by a vector  $a \in \mathbb{R}^n$ . We can rewrite the two alternatives depending on whether  $u(a)$  is zero or not, as follows:

- (1) If  $u(a) \neq 0$ : for every  $p \in I$ , we have  $\varphi(p) = \frac{p(a)}{u(a)}$ .
- (2) If  $u(a) = 0$ : for every  $p \in \mathbb{R}[x]$  and every  $q \in I$ , we have  $\varphi(pq) = p(a)\varphi(q)$ .

We first show that in both cases  $a$  belongs to  $S(M)$ . Indeed, let  $p \in M$ . We have  $pu \in I \cap M$ , since  $uM \subseteq M$ . Then, (in both cases) we have  $\varphi(pu) = p(a) \geq 0$ .

Assume now that we are the case (2). Since  $u, f \in I$ , we can compute  $\varphi(fu)$  in two ways. First, we have  $\varphi(fu) = \varphi(f)u(a) = 0$ . Also,  $\varphi(fu) = f(a)\varphi(u) = f(a)$ . Hence,  $f(a) = 0$ , so  $a \in Z(f)$ , so that  $a \in Z(f) \cap S(M)$ . Hence,  $\varphi$  is precisely a test state on  $I$  for  $M$  at a point in  $Z(f) \cap S(M)$ , so that  $\varphi(f) > 0$  by assumption.

Finally, assume that we are in case (1), i.e.,  $u(a) \neq 0$ . Then we have  $u(a) > 0$ , because  $u \in M$  and  $a \in S(M)$ . By assumption  $f \geq 0$  on  $S(M)$ , so we have  $f(a) \geq 0$ . Also, by assumption, we have  $Z(f) \cap S(M) \subseteq Z(u) \cap S(M)$ . This shows that, whenever  $u(a) \neq 0$ , we have  $\varphi(f) = \frac{f(a)}{u(a)} > 0$ . Then, in case (1) we also have  $\varphi(f) > 0$ , concluding the proof.  $\square$

**Remark 6.23.** *Observe that Theorem 6.22 implies Putinar's Positivstellensatz (Theorem 1.9). Suppose  $M$  is an Archimedean quadratic module and assume that  $f > 0$  on  $S(M)$ . We set  $I = \mathbb{R}[x]$  the ideal generated by the constant polynomial  $u = 1$ . So that  $\mathfrak{g} = \{1\}$ . Clearly,  $Z(f) \cap S(M) = \emptyset = Z(1) \cap S(M)$ ,  $uM = M$ , and the polynomial  $u = 1$  is  $\mathfrak{g}$ -stably contained in  $M$ . Finally, the test state condition follows trivially because  $Z(f) \cap S(M)$  is empty so there are no such test states.*

### 6.3. Positive diagonal scalings of the Horn matrix

This section is devoted to the proof of Theorem 6.3. For this, we will apply Theorem 6.22 in a special setting. We start with a preliminary result that will be used in the proof of Theorem 6.3. This result is a reformulation of Theorem 5.6, in which we characterized the diagonal scalings of the Horn matrix that belong to the cone  $\mathcal{K}_5^{(1)}$ .

**Lemma 6.24.** *Let  $d_1, d_2, \dots, d_5 > 0$ , then*

$$\left(\sum_{i=1}^5 d_i x_i^2\right)(x^{\circ 2})^\top H x^{\circ 2} \in \Sigma, \quad \text{if and only if} \quad (6.6)$$

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

PROOF. This follows directly from Theorem 5.6 after rescaling the variables.  $\square$

We will just use the “if” part of Lemma 6.24 that also follows from the following explicit decomposition (which can be found by using the explicit  $\mathcal{K}^{(1)}$ -certificate for the diagonal scalings of the Horn matrix found in Theorem 5.6):

$$\begin{aligned} \left(\sum_{i=1}^5 d_i x_i^2\right)(x^{\circ 2})^\top H x^{\circ 2} &= d_1 x_1^2 (x_1^2 + x_2^2 + x_5^2 - x_3^2 - x_4^2)^2 \\ &\quad + d_2 x_2^2 (x_1^2 + x_2^2 + x_3^2 - x_4^2 - x_5^2)^2 \\ &\quad + d_3 x_3^2 (x_2^2 + x_3^2 + x_4^2 - x_5^2 - x_1^2)^2 \\ &\quad + d_4 x_4^2 (x_3^2 + x_4^2 + x_5^2 - x_1^2 - x_2^2)^2 \\ &\quad + d_5 x_5^2 (x_1^2 + x_4^2 + x_5^2 - x_2^2 - x_3^2)^2 \\ &\quad + 4x_1^2 x_2^2 x_5^2 (d_5 - d_1 + d_2) + 4x_1^2 x_2^2 x_3^2 (d_3 + d_1 - d_2) \\ &\quad + 4x_2^2 x_3^2 x_4^2 (d_4 + d_2 - d_3) + 4x_3^2 x_4^2 x_5^2 (d_5 + d_3 - d_4) \\ &\quad + 4x_4^2 x_5^2 x_1^2 (d_1 + d_4 - d_5). \end{aligned}$$

In particular, if  $(d_1, d_2, \dots, d_5) \approx (1, 1, \dots, 1)$ , then  $(\sum_{i=1}^5 d_i x_i^2)(x^{\circ 2})^\top H x^{\circ 2}$  is a sum of squares.

Now we proceed with the proof of Theorem 6.3.

**Proof of Theorem 6.3.** We observe that relation (6.4) in Theorem 6.3 holds for any  $d_1, \dots, d_5 > 0$  if and only if for any  $d_1, \dots, d_5 > 0$  we have

$$(x^{\circ 2})^\top H x^{\circ 2} \in \Sigma + I\left(\sum_{i=1}^5 d_i x_i^2 - 1\right). \quad (6.7)$$



We set  $h := (x^{\circ 2})^\top H x^{\circ 2}$ . We will show that relation (6.7) holds by applying Theorem 6.22 in the following setting:

- $M = \Sigma + I\left(\sum_{i=1}^5 d_i x_i^2 - 1\right)$
- $I = I(h)$ , so it is generated by the set  $\mathbf{g} = \{h\}$ .
- $u = \left(\sum_{i=1}^5 x_i^2\right)h$
- $f = h$

In what follows we will show that this setting satisfies the assumptions of Theorem 6.22, thus enabling us to conclude that  $h \in M$ , as desired. First, we show that  $M$  is Archimedean. We have  $1 - \sum_{i=1}^5 d_i x_i^2 \in M$ . If we set  $d = \min\{d_i : i \in [5]\}$ , then we have  $1 - \sum_{i=1}^5 d x_i \in M$ , so that  $\frac{1}{d} - \sum_{i=1}^5 x_i^2 \in M$ . Thus, for any  $N > \frac{1}{d}$ , we have  $N - \sum_{i=1}^5 x_i^2 \in M$ . Since  $H$  is copositive we have that  $h$  is globally nonnegative. In particular,  $h \geq 0$  on  $S(M)$ . Clearly, we have  $Z(h) \cap S(M) \subseteq Z(u) \cap S(M)$ , and  $uM \subseteq M$  holds as  $u \in \Sigma$  (since  $H \in \mathcal{K}_5^{(1)}$ ).

We now show that  $\left(\sum_{i=1}^5 x_i^2\right)h$  is  $\mathbf{g}$ -stably contained in  $M$ . By relation (6.6), the polynomial  $\sigma := \left(\sum_{i=1}^5 x_i^2 \pm \varepsilon \sum_{i=1}^5 d_i x_i^2\right)h$  is a sum of squares for some  $\varepsilon > 0$  small enough. Then,

$$\begin{aligned}\sigma &= \left(\sum_{i=1}^5 x_i^2\right)h \pm \varepsilon \left(\sum_{i=1}^5 d_i x_i^2\right)h, \\ \sigma &= \left(\sum_{i=1}^5 x_i^2\right)h \pm \varepsilon \left(\sum_{i=1}^5 d_i x_i^2 - 1 + 1\right)h,\end{aligned}$$

$$\text{which implies } \left(\sum_{i=1}^5 x_i^2\right)h \pm \varepsilon h = \sigma \mp \varepsilon \left(\sum_{i=1}^5 d_i x_i^2 - 1\right)h \in M,$$

showing that  $\left(\sum_{i=1}^5 x_i^2\right)h$  is  $\mathbf{g}$ -stably contained in  $M$ . It remains to show that for all test states  $\varphi$  on  $I$  for  $M$  at a point  $a \in Z(h) \cap S(M)$  with respect to  $u$ , we have  $\varphi(h) > 0$ . Let  $\varphi$  be such state. Then, we have

$$\varphi\left(\left(\sum_{i=1}^5 x_i^2\right)h\right) = 1 = \left(\sum_{i=1}^5 a_i^2\right)\varphi(h).$$

This shows that  $\varphi(h) > 0$  as  $a \neq 0$ . Then, by Theorem 6.22, we have that  $h = (x^{\circ 2})^\top H x^{\circ 2} \in M$ .

#### 6.4. The hierarchy $\vartheta^{(r)}(G)$ has finite convergence

In this section, we show Theorem 6.4 that, as mentioned earlier, implies the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  for every graph  $G$ .

**Proof of Theorem 6.4.** Recall that, by assumption,  $\vartheta\text{-rank}(G) < \infty$ . Then, there exists  $r \in \mathbb{N}$  such that  $(\sum_{i=1}^n x_i^2)^r f_G \in \Sigma$ . We fix  $\alpha := \alpha(G)$ , so that  $\alpha(G \oplus i_0) = \alpha + 1$ . Observe that the following identity holds (this also follows from relation (5.13), see also [GL07]):

$$f_{G \oplus i_0} = g^2 + \frac{\alpha + 1}{\alpha} f_G, \text{ where } g := \sqrt{\alpha} x_{i_0}^2 - \frac{1}{\sqrt{\alpha}} (x_1^2 + \dots + x_n^2). \quad (6.8)$$

Indeed, we compare coefficients

$$\begin{aligned} x_{i_0}^4 &: \alpha = \alpha \\ x_i^4 \text{ for } (i \neq i_0) &: \alpha = \frac{1}{\alpha} + \frac{\alpha + 1}{\alpha} \cdot (\alpha - 1) \\ x_i^2 x_j^2 \text{ for } \{i, j\} \in E &: 2\alpha = \frac{2}{\alpha} + \frac{\alpha + 1}{\alpha} \cdot 2(\alpha - 1) \\ x_i^2 x_j^2 \text{ for } \{i, j\} \notin E, i, j \neq i_0 &: -2 = \frac{2}{\alpha} - 2 \cdot \frac{\alpha + 1}{\alpha} \\ x_{i_0}^2 x_i^2 \text{ for } i \neq i_0 &: -2 = -2 \cdot \frac{\sqrt{\alpha}}{\sqrt{\alpha}} \end{aligned}$$

We apply Theorem 6.22 in the following setting:

- $M := \Sigma + I\left(x_{i_0}^2 + \sum_{i=1}^n x_i^2 - 1\right)$ ,
- $I := I(\{g^2, f_G\})$ ,
- $u := \underbrace{g^2}_{=:u_1} + \underbrace{\frac{\alpha + 1}{\alpha} \left(\sum_{i=1}^n x_i^2\right)^{2r}}_{=:u_2} f_G$ ,
- $f = f_{G \oplus i_0}$ .

Then,  $M$  is Archimedean,  $f \in I$ , and  $u \in M \cap I$ . Clearly,  $f_{G \oplus i_0} \geq 0$  on  $S(M)$ , because  $f_{G \oplus i_0}$  is globally nonnegative (as  $M_{G \oplus i_0}$  is copositive). Now, by looking at relation (6.8), if  $f_{G \oplus i_0}(x) = 0$ , then  $g^2(x) = 0$  and  $f_G(x) = 0$ . This implies

$$Z(f_{G \oplus i_0}) \subseteq Z(u),$$

and thus,

$$Z(f_{G \oplus i_0}) \cap S(M) \subseteq Z(u) \cap S(M).$$

The inclusion  $uM \subseteq M$  holds as  $u \in \Sigma$  (by construction). Now, we show that  $u$  is  $\mathfrak{g}$ -stably contained in  $M$ . First, it is clear that  $u \pm g^2$  is a sum of squares, so it belongs to  $M$ . It remains to prove that there exists  $\varepsilon > 0$  such that  $u \pm \varepsilon f_G \in M$ , which is equivalent to show that there exists  $N > 0$  such that  $Nu \pm f_G \in M$ . For this, we will show the following two statements.

- (1) There exist  $N_1, N_2 \in \mathbb{N}$  such that  $N_1 u_1 + N_2 u_2 + f_G \in M$ ,
- (2) There exist  $N_1, N_2 \in \mathbb{N}$  such that  $N_1 u_1 + N_2 u_2 - f_G \in M$ ,

If this holds, then using that  $u_1, u_2 \in \Sigma \subseteq M$ , we obtain that there exists  $N \in \mathbb{N}$  such that  $Nu \pm f_G \in M$ , as desired.

For proving (1) and (2), observe that if we have  $p_1 \equiv p_2 \pmod{x_{i_0}^2 + \sum_{i=1}^n x_i^2 - 1}$ , then  $p_1 \in M$  if and only if  $p_2 \in M$ . We have the following:

$$1 - x_{i_0}^2 \equiv \sum_{i=1}^n x_i^2 \pmod{x_{i_0}^2 + \sum_{i=1}^n x_i^2 - 1}, \quad (6.9)$$

$$g \equiv \frac{1}{\sqrt{\alpha}}((\alpha + 1)x_{i_0}^2 - 1) \pmod{x_{i_0}^2 + \sum_{i=1}^n x_i^2 - 1}. \quad (6.10)$$

**Proof of (1):** Consider the univariate polynomial  $p := c'(1 - x_{i_0}^2)^r - 1$  in  $\mathbb{R}[x_{i_0}]$ , where  $c' := (1 - \frac{1}{\alpha+1})^{-r}$ . Observe that  $x_{i_0} = \pm \frac{1}{\sqrt{\alpha+1}}$  are roots of  $p$ . Thus,  $(\alpha + 1)x_{i_0}^2 - 1$  divides  $p$  in  $\mathbb{R}[x_{i_0}]$ , so we can write

$$p = ((\alpha + 1)x_{i_0}^2 - 1)q$$

for some  $q \in \mathbb{R}[x_{i_0}]$ . Since  $M$  is Archimedean, using Definition 6.13, there exists  $C \in \mathbb{N}$  such that

$$C + q^2 f_G \in M.$$

Since  $((\alpha + 1)x_{i_0}^2 - 1)^2 \in \Sigma$  and  $\Sigma M \subseteq M$ , we have

$$C((\alpha + 1)x_{i_0}^2 - 1)^2 + p^2 f_G = (C + q^2 f_G)((\alpha + 1)x_{i_0}^2 - 1)^2 \in M.$$

Then, by using the definition of  $p$ , we obtain

$$C((\alpha + 1)x_{i_0}^2 - 1)^2 + c'^2(1 - x_{i_0}^2)^{2r} f_G - 2c'(1 - x_{i_0}^2)^r f_G + f_G \in M.$$

Using (6.10) and (6.9) we obtain

$$\alpha C g^2 + c'^2 \left( \sum_{i=1}^n x_i^2 \right)^{2r} f_G - 2c' \left( \sum_{i=1}^n x_i^2 \right)^r f_G + f_G \in M.$$

By assumption, we have that  $(\sum_{i=1}^n x_i^2)^r f_G \in \Sigma \subseteq M$  and thus

$$\alpha C g^2 + c'^2 \left( \sum_{i=1}^n x_i^2 \right)^{2r} f_G + f_G \in M,$$

which shows (1).

**Proof of (2):** Consider the univariate polynomial  $p := c'(1 - x_{i_0}^2)^{2r} - 1$  in  $\mathbb{R}[x_{i_0}]$ , where  $c' := (1 - \frac{1}{\alpha+1})^{-2r}$ . Observe that  $x_{i_0} = \pm \frac{1}{\sqrt{\alpha+1}}$  are roots of  $p$ . Thus,  $(\alpha + 1)x_{i_0}^2 - 1$  divides  $p$  in  $\mathbb{R}[x_{i_0}]$ , so we can write

$$p = ((\alpha + 1)x_{i_0}^2 - 1)q$$

for some  $q \in \mathbb{R}[x_{i_0}]$ . Since  $M$  is Archimedean, there exists  $C \in \mathbb{N}$  such that

$$C - q^2 f_G \in M.$$

Since  $((\alpha + 1)x_{i_0}^2 - 1)^2 \in \Sigma \subseteq M$  and  $\Sigma M \subseteq M$  we have

$$C((\alpha + 1)x_{i_0}^2 - 1)^2 - p^2 f_G = ((\alpha + 1)x_{i_0}^2 - 1)^2 (C - q^2 f_G) \in M.$$

That is,

$$C((\alpha + 1)x_{i_0}^2 - 1)^2 - c'^2(1 - x_{i_0}^2)^{4r} f_G + 2c'(1 - x_{i_0}^2)^{2r} f_G - f_G \in M.$$

Using (6.10) and (6.9), we obtain

$$\alpha Cg^2 - c'^2 \left( \sum_{i=1}^n x_i^2 \right)^{4r} f_G + 2c' \left( \sum_{i=1}^n x_i^2 \right)^{2r} f_G - f_G \in M.$$

By assumption, we have  $(\sum_{i=1}^n x_i^2)^r f_G \in \Sigma$ . This implies  $(\sum_{i=1}^n x_i^2)^{4r} f_G \in \Sigma$ . Hence, we have

$$\alpha Cg^2 + 2c' \left( \sum_{i=1}^n x_i^2 \right)^{2r} f_G - f_G \in M,$$

which shows (2).

Finally, we check the test state property. Let  $\varphi$  be a test state on  $I$  for  $M$  at a point  $a \in Z(f_{G \oplus i_0}) \cap S(M)$  with respect to  $u$ . Since  $(\sum_{i=1}^n x_i^2)^r f_G \in M \cap I$ , we have that

$$0 \leq \varphi \left( \left( \sum_{i=1}^n x_i^2 \right)^r f_G \right) = \left( \sum_{i=1}^n a_i^2 \right)^r \varphi(f_G),$$

where  $a_{i_0}^2 + \sum_{i=1}^n a_i^2 = 1$  (recall Remark 6.21) and  $f_{G \oplus i_0}(a) = 0$ . It is easy to observe that  $f_{G \oplus i_0}(\pm 1, 0, \dots, 0) > 0$ , so that  $a \neq (\pm 1, \dots, 0)$ . This implies that  $\sum_{i=1}^n a_i^2 > 0$ , and thus  $\varphi(f_G) \geq 0$ . Since  $g^2 \in I \cap M$ , we have that  $\varphi(g^2) \geq 0$ . Also, we have

$$\begin{aligned} 1 = \varphi(u) &= \varphi(g^2) + \frac{\alpha + 1}{\alpha} \varphi \left( \left( \sum_{i=1}^n x_i^2 \right)^{2r} f_G \right) \\ &= \varphi(g^2) + \frac{\alpha + 1}{\alpha} \left( \sum_{i=1}^n a_i^2 \right)^{2r} \varphi(f_G). \end{aligned}$$

Therefore,  $\varphi(g^2)$  and  $\varphi(f_G)$  are nonnegative but they cannot be both zero. Using relation (6.8), we obtain

$$\varphi(f_{G \oplus i_0}) = \varphi(g^2) + \frac{\alpha + 1}{\alpha} \varphi(f_G) > 0,$$

as desired.

## CHAPTER 7

# Bicliques and biindependent sets

*This chapter is based on my work [LPV23] with Monique Laurent and Sven Polak.*

Given a bipartite graph  $G = (V_1 \cup V_2, E)$ , a *bipartite biindependent pair* in  $G$  is a pair  $(A, B)$  of subsets  $A \subseteq V_1$  and  $B \subseteq V_2$  such that no pair of nodes  $\{i, j\} \in A \times B$  is an edge of  $G$ . The adjective “bipartite” is used to indicate that we restrict to the pairs  $(A, B)$  that respect the bipartite structure of  $G$ , i.e., with  $A \subseteq V_1$  and  $B \subseteq V_2$ ; we will however sometimes omit it for the sake of brevity. The maximum sum  $|A| + |B|$  taken over all bipartite biindependent pairs  $(A, B)$  is the well-studied parameter  $\alpha(G)$ . We consider the following two other parameters, asking for the maximum product  $|A| \cdot |B|$  and the maximum ratio  $\frac{|A| \cdot |B|}{|A| + |B|}$ ,

$$g(G) := \max\{|A| \cdot |B| : (A, B) \text{ is a bipartite biindependent pair in } G\}, \quad (7.1)$$

$$h(G) := \max\left\{\frac{|A| \cdot |B|}{|A| + |B|} : (A, B) \text{ is a bipartite biindependent pair in } G\right\}. \quad (7.2)$$

If  $G$  is a complete bipartite graph, then any bipartite biindependent pair has  $A = \emptyset$  or  $B = \emptyset$  (and thus  $g(G) = h(G) = 0$ ); such a pair is called *trivial*. Otherwise, in the definition of  $g(G)$  and  $h(G)$ , one may restrict the optimization to *nontrivial* pairs  $(A, B)$ , i.e., with  $A, B \neq \emptyset$ . A pair  $(A, B)$  is called *balanced* if  $|A| = |B|$ . Then a related parameter of interest is  $\alpha_{\text{bal}}(G)$ , the maximum number of vertices in a balanced biindependent pair, given by

$$\alpha_{\text{bal}}(G) := \max\{|A| + |B| : (A, B) \text{ is a balanced biindependent pair in } G\}.$$

One can also define the parameters  $g_{\text{bal}}(G)$  and  $h_{\text{bal}}(G)$  as the analogs of  $g(G)$  and  $h(G)$ , where one restricts the optimization to balanced pairs in (7.1) and (7.2), respectively.

### 7.1. Introduction

In this section we first present a first introductory result that relates the parameters defined above. Then, we explain some applications of the parameters. Next, we present a roadmap through the main results of the chapter, that deal with complexity questions, and with designing semidefinite bounds and closed-form eigenvalue-based bounds, topics to which we come back in detail in Sections 7.2, 7.3, 7.4, and 7.6. In Section 7.5 we will present several

illustrating examples.

We have the following easy relations among the above parameters.

**Lemma 7.1.** *Let  $G$  be a bipartite graph. Then, we have*

$$\frac{1}{4}\alpha_{\text{bal}}(G) = \frac{1}{2}\sqrt{g_{\text{bal}}(G)} = h_{\text{bal}}(G) \leq h(G) \leq \frac{1}{2}\sqrt{g(G)} \leq \frac{1}{4}\alpha(G), \quad (7.3)$$

$$h(G) = \frac{1}{4}\alpha(G) \iff \frac{1}{2}\sqrt{g(G)} = \frac{1}{4}\alpha(G) \iff \alpha(G) = \alpha_{\text{bal}}(G), \quad (7.4)$$

PROOF. The equalities  $\frac{1}{4}\alpha_{\text{bal}}(G) = \frac{1}{2}\sqrt{g_{\text{bal}}(G)} = h_{\text{bal}}(G)$  follow from the definitions. We now show the inequalities in (7.3). First, if  $(A, B)$  is optimal for  $\alpha_{\text{bal}}(G)$ , then  $|A| = |B|$  and thus we have  $h(G) \geq \frac{|A| \cdot |B|}{|A| + |B|} = |A|/2 = \alpha_{\text{bal}}(G)/4$ . Second, if  $(A, B)$  is optimal for  $h(G)$ , then  $\frac{1}{2}\sqrt{g(G)} \geq \frac{1}{2}\sqrt{|A| \cdot |B|} \geq \frac{|A| \cdot |B|}{|A| + |B|} = h(G)$ , where the last inequality holds as  $(\sqrt{|A|} - \sqrt{|B|})^2 \geq 0$ . Third, if  $(A, B)$  is optimal for  $g(G)$ , then  $\frac{1}{4}\alpha(G) \geq \frac{1}{4}(|A| + |B|) \geq \frac{1}{2}\sqrt{|A| \cdot |B|} = \frac{1}{2}\sqrt{g(G)}$ , where again the last inequality holds as  $(\sqrt{|A|} - \sqrt{|B|})^2 \geq 0$ . This concludes the proof of (7.3). Moreover, equality  $\frac{1}{4}\alpha(G) = \frac{1}{2}\sqrt{g(G)}$  implies  $|A| = |B|$ , and thus  $(A, B)$  is a balanced optimal solution for  $\alpha(G)$ , so that  $\alpha(G) = \alpha_{\text{bal}}(G)$ . In addition, if  $h(G) = \frac{1}{4}\alpha(G)$ , then  $\frac{1}{4}\alpha(G) = \frac{1}{2}\sqrt{g(G)}$  by (7.3), which, as we just observed, implies  $\alpha(G) = \alpha_{\text{bal}}(G)$ . The other implications follow directly from (7.3).  $\square$

Now, we explain how the above parameters also permit to model problems about bicliques (in arbitrary graphs) and we mention some applications.

**Biindependent pairs and bicliques in arbitrary graphs.** *Bipartite* biindependent pairs in *bipartite* graphs also permit to model *general* biindependent pairs and bicliques in *arbitrary* graphs. Consider an arbitrary graph  $G = (V, E)$  (not necessarily bipartite). A *biindependent* pair in  $G$  is a pair  $(A, B)$  of disjoint subsets of  $V$  such that no pair of nodes  $\{i, j\} \in A \times B$  is an edge of  $G$  (but edges are allowed within  $A$  or  $B$ ). One then defines analogously the parameters  $g_{\text{bi}}(G)$  and  $h_{\text{bi}}(G)$ , respectively, as the maximum product  $|A| \cdot |B|$  and the maximum ratio  $\frac{|A| \cdot |B|}{|A| + |B|}$ , taken over all biindependent pairs in  $G$ . The analog of relation (7.3) holds:

$$h_{\text{bi}}(G) \leq \frac{1}{2}\sqrt{g_{\text{bi}}(G)} \leq \frac{1}{4}|V|.$$

Note that  $h_{\text{bi}}(G) \geq \frac{1}{4}\alpha(G)$  if  $\alpha(G)$  is even and  $h_{\text{bi}}(G) \geq \frac{1}{4}(\alpha(G) - \frac{1}{\alpha(G)})$  if  $\alpha(G)$  is odd (which can be seen by partitioning a maximum stable set into two almost equally sized parts). The parameters  $h_{\text{bi}}(G)$  and  $g_{\text{bi}}(G)$  can in fact be reformulated in terms of the parameters  $g(\cdot)$  and  $h(\cdot)$  for an associated bipartite graph  $B_0(G)$ , the *extended bipartite double* of  $G$ , defined as follows. First we define the *bipartite double*  $B(G)$ , whose node set is  $V \cup V'$ , where

$V' = \{i' : i \in V\}$  is a disjoint copy of  $V$ , and whose edges are the pairs  $\{i, j'\}$  and  $\{j, i'\}$  for  $\{i, j\} \in E$ . Then, the *extended bipartite double*  $B_0(G)$  is obtained by adding all pairs  $\{i, i'\}$  ( $i \in V$ ) as edges to  $B(G)$ . Now, observe that a pair  $(A, B)$  is biindependent in  $G$  precisely when the pair  $(A \subseteq V, B' := \{i' : i \in B\} \subseteq V')$  is bipartite biindependent in  $B_0(G)$ . Therefore we have

$$g_{\text{bi}}(G) = g(B_0(G)) \quad \text{and} \quad h_{\text{bi}}(G) = h(B_0(G)) \quad \text{for any graph } G. \quad (7.5)$$

One can also model bicliques in an arbitrary graph  $G = (V, E)$ . A *biclique* in  $G$  is a pair  $(A, B)$  of disjoint subsets of  $V$  such that  $A \times B \subseteq E$  or, equivalently,  $(A, B)$  is a biindependent pair in the complementary graph  $\overline{G} = (V, \overline{E})$  of  $G$ . In analogy, let  $g_{\text{bc}}(G)$  and  $h_{\text{bc}}(G)$  denote the maximum product  $|A| \cdot |B|$  and ratio  $\frac{|A| \cdot |B|}{|A| + |B|}$ , taken over all bicliques  $(A, B)$  in  $G$ , so that for any graph  $G$  we have

$$g_{\text{bc}}(G) = g_{\text{bi}}(\overline{G}) = g(B_0(\overline{G})) \quad \text{and} \quad h_{\text{bc}}(G) = h_{\text{bi}}(\overline{G}) = h(B_0(\overline{G})). \quad (7.6)$$

In the case when  $G = (V_1 \cup V_2, E)$  is a bipartite graph, nontrivial bicliques in  $G$  correspond to nontrivial bipartite biindependent pairs in the bipartite graph  $\overline{G}^b := (V_1 \cup V_2, (V_1 \times V_2) \setminus E)$ , known as the *bipartite complement* of  $G$ . So we also have

$$g_{\text{bc}}(G) = g(\overline{G}^b) \quad \text{and} \quad h_{\text{bc}}(G) = h(\overline{G}^b) \quad \text{for any graph } G. \quad (7.7)$$

So relations (7.6) and (7.7) offer different formulations for the parameters  $g_{\text{bc}}(\cdot)$  and  $h_{\text{bc}}(\cdot)$ , we will investigate in Section 7.4.3 how the associated semidefinite bounds relate.

**Complexity results.** As is well-known, there are polynomial-time algorithms for computing the stability number  $\alpha(G)$  of a bipartite graph  $G$ . For example, by computing  $\vartheta(G)$  (which is equal to  $\alpha(G)$ , as  $G$  is perfect) with precision  $\frac{1}{4}$ . On the other hand, Peeters [Pe03] shows that, given an integer  $k$ , deciding whether a bipartite graph  $G$  has a biclique  $(A, B)$  with  $|A| \cdot |B| \geq k$  is an NP-complete problem. Hence, computing the parameter  $g(G)$  is an NP-hard problem (by switching between bicliques and biindependent pairs).

We will show that also  $h(G)$  is hard to compute. For this, we show that the problem (denoted  $\alpha$ -BAL-BIP in Section 7.2) of deciding whether a bipartite graph  $G$  has a *balanced* maximum independent set, i.e., whether it holds that  $\alpha(G) = \alpha_{\text{bal}}(G)$ , is NP-complete (see Theorem 7.4). Combining with Lemma 7.1, it follows that deciding whether  $h(G) \geq \frac{1}{4}\alpha(G)$  is an NP-complete problem.

It is known that, given an integer  $k$ , deciding whether a bipartite graph  $G$  contains a bipartite biindependent pair  $(A, B)$  with  $|A| = |B| = k$  is an NP-complete problem [Gar79, John87] (switching between biindependent pairs and bicliques). Hence our hardness result for problem  $\alpha$ -BAL-BIP shows hardness of this problem already for the case  $k = \frac{1}{2}\alpha(G)$ .

Our proof technique will in fact permit to show NP-hardness for a broader set of problems, namely for deciding whether any of the following equalities holds:  $g(G) = g_{\text{bal}}(G)$ ,  $h(G) = h_{\text{bal}}(G)$ ,  $h(G) = \frac{1}{2}\sqrt{g(G)}$ , or  $\frac{1}{2}\sqrt{g(G)} = \frac{1}{4}\alpha(G)$  (thus whether the inequalities in (7.3) hold at equality). See Theorem 7.11 and Corollary 7.12.

**Some applications for the parameters  $g(\cdot)$  and  $h(\cdot)$ .** As explained above, the parameter  $g(\cdot)$  also allows to model maximum edge cardinality bicliques in bipartite (or general) graphs. This problem has many real life applications, such as reducing assembly times in product manufacturing lines and in the area of formal concept analysis, as explained in [DKST01] (see also [DKT97, ST98]). The related parameter asking for the maximum number of vertices in a balanced biclique has also many applications; e.g., in VLSI design (e.g., [AYRP07, RL88, Tah06]), in the analysis of biological data (as instance of bicluster, e.g., [YWWY05]) and of interactions of proteins (e.g., [MRU87]).

The parameter  $g(\cdot)$  is also relevant for bounding the nonnegative rank of a matrix. Given a matrix  $M \in \mathbb{R}_+^{|V_1| \times |V_2|}$ , its *nonnegative rank*  $\text{rank}_+(M)$  is the smallest integer  $r \in \mathbb{N}$  such that  $M = \sum_{\ell=1}^r a_\ell b_\ell^\top$  for some nonnegative vectors  $a_\ell \in \mathbb{R}_+^{|V_1|}$  and  $b_\ell \in \mathbb{R}_+^{|V_2|}$ ; computing  $\text{rank}_+(\cdot)$  is an NP-hard problem [Vav09]. A classical combinatorial lower bound for  $\text{rank}_+(M)$  is the *rectangle covering bound*  $\text{rc}(M)$ , defined as the smallest number of rectangles  $A \times B \subseteq V_1 \times V_2$  whose union is equal to the support  $S_M := \{(i, j) \in V_1 \times V_2 : M_{ij} \neq 0\}$  of  $M$ . (See, e.g., [FKPT13]). The rectangle covering bound was used, e.g., in [FMPTW12] to show an exponential lower bound on the extension complexity of combinatorial polytopes such as the traveling salesman and correlation polytopes. Also the parameter  $\text{rc}(M)$  is not easy to compute. To approximate it, one can consider the bipartite graph  $B_M$ , with vertex set  $V_1 \cup V_2$  and edge set  $E_M := (V_1 \times V_2) \setminus S_M$ . Then one can show that  $\text{rc}(M) \cdot g(B_M) \geq |S_M|$ . Hence, an upper bound on  $g(B_M)$  gives directly a lower bound on  $\text{rc}(M)$  and thus a lower bound on the nonnegative rank  $\text{rank}_+(M)$ .

The parameter  $h(\cdot)$  was introduced by Vallentin [Val20], who observed its relevance to maximum product-free subsets in groups in work of Gowfers [Gow08]. Let  $\Gamma$  be a finite group. A set  $A \subseteq \Gamma$  is called *product-free* if  $ab \notin A$  for every pair of elements  $a, b \in A$ , and one is interested in finding the largest cardinality of a product-free set in  $\Gamma$  (see [Gow08, Ked09] for background on this problem). We now briefly indicate how to bound this parameter using the parameter  $h(\cdot)$ ; for the interested reader we present this connection in more detail in my work with Laurent and Polak [LPV23, Appendix A].

Assume  $A \subseteq \Gamma$  is product-free. Let  $G_{\Gamma, A} = (V_1 \cup V_2, E)$  be the associated bipartite Cayley graph, where  $V_1$  and  $V_2$  are disjoint copies of  $\Gamma$  and there is an edge between  $v_1 \in V_1$  and  $v_2 \in V_2$  if their product  $v_1 v_2$  belongs to  $A$ . The



crucial observation now is that since  $A$  is product-free, the pair  $(A_1, A_2)$  is (balanced) bipartite biindependent in  $G_{\Gamma, A}$ , where  $A_1 \subseteq V_1, A_2 \subseteq V_2$  are the corresponding disjoint copies of  $A$ . This implies  $\frac{|A|}{2} \leq h(G_{\Gamma, A})$ . Hence, upper bounds on  $h(G_{\Gamma, A})$  give upper bounds on product-free sets in  $\Gamma$ . Vallentin [Val20] introduced the eigenvalue-based upper bound  $h(G) \leq \frac{|V|}{2r} \lambda_2(A_G)$  for any  $r$ -regular bipartite graph  $G$ . Applying it to the  $|A|$ -regular bipartite graph  $G_{\Gamma, A}$ , he could recover a result by Gowers [Gow08], which states that a product-free subset  $A$  in  $\Gamma$  has cardinality  $|A| \leq |\Gamma|/k^{1/3}$ , where  $k$  is the minimum dimension of a nontrivial representation of  $\Gamma$ . We will show the sharper eigenvalue-based bound  $h(G) \leq \widehat{h}(G) = \frac{|V|}{4} \frac{\lambda_2(A_G)}{r + \lambda(A_G)}$  (see Proposition 7.22). This gives a slight sharpening of Gowers' bound, replacing  $\frac{|\Gamma|}{k^{1/3}}$  by  $\frac{|\Gamma|}{1+k^{1/3}}$  (see Theorem A.2 in [LPV23]).

In fact, for this application, one is only interested in *balanced* biindependent pairs in the graph  $G_{\Gamma, A}$  and we have  $2|A| \leq \alpha_{\text{bal}}(G_A)$  if  $A$  is product-free in  $\Gamma$ . This motivates investigating whether sharper semidefinite and eigenvalue-based bounds can be found for the balanced parameters. We come back briefly to this question later in the introduction and it will be investigated in detail in Section 7.6.

**Semidefinite approximations.** The parameters  $g(G)$  and  $h(G)$  can be formulated as polynomial optimization problems, which leads to hierarchies of semidefinite programming (SDP) upper bounds  $g_r(G)$  and  $h_r(G)$  (for  $r \geq 1$ ), able to find the original parameters at order  $r = \alpha(G)$ . We investigate in particular the SDP bounds obtained at the first order  $r = 1$ . As we will see they take the form

$$g_1(G) = \max_{X \in \mathcal{S}^V} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^T \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, X_{ij} = 0 \text{ if } \{i, j\} \in E \right\}, \quad (7.8)$$

$$h_1(G) = \max_{X \in \mathcal{S}^V} \{ \langle C, X \rangle : X \succeq 0, \text{Tr}(X) = 1, X_{ij} = 0 \text{ if } \{i, j\} \in E \}. \quad (7.9)$$

Here,  $C = \frac{1}{2} \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} \in \mathbb{R}^{|V_1|+|V_2|}$ , where  $J$  denotes the all-ones matrix of appropriate size. The parameters  $g_1(G)$  and  $h_1(G)$  can be seen as quadratic variations of the parameter  $\vartheta(G)$  (which, if  $G$  is bipartite (and thus perfect), is equal to  $\alpha(G)$ ). Indeed, If we replace  $\langle C, X \rangle$  by  $\langle J, X \rangle$  in program (7.9) we obtain the formulation (3.1) for  $\vartheta(G)$  introduced in Chapter 3. If we replace the objective  $\langle C, X \rangle$  by  $\text{Tr}(X)$  in program (7.8), then we obtain another well-known formulation for  $\vartheta(G)$ , see formulation (7.20). We will show the following relations between the parameters  $h(G)$ ,  $g(G)$ ,  $h_1(G)$ ,  $g_1(G)$ , and  $\alpha(G)$ .

**Proposition 7.2.** *For any bipartite graph  $G$  we have*

$$h(G) \leq \frac{1}{2} \sqrt{g(G)} \leq h_1(G) \leq \frac{1}{2} \sqrt{g_1(G)} \leq \frac{1}{4} \alpha(G).$$

It is interesting to note that  $h_1(G)$  may improve the bound  $\frac{1}{2}\sqrt{g_1(G)}$  for  $\frac{1}{2}\sqrt{g(G)}$ . Indeed, the inequality  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$  can be strict, e.g., when  $G$  is  $K_{n,n}$  minus a perfect matching with  $n \geq 5$ , as we see in Section 7.5. The key ingredient to show this is getting eigenvalue-based reformulations for the parameters when  $G$  enjoys symmetry properties, as we discuss next.

**Eigenvalue bounds.** When  $G$  is a bipartite  $r$ -regular graph we can give closed-form bounds in terms of the second largest eigenvalue of the adjacency matrix  $A_G$  of  $G$ . These bounds are obtained by restricting in the definitions (7.8) and (7.9) of  $g_1(G)$  and  $h_1(G)$  the optimization to matrices with some symmetry.

**Proposition 7.3.** *Assume  $G$  is a bipartite  $r$ -regular graph, set  $n := |V_1| = |V_2|$ , and let  $\lambda_2$  be the second largest eigenvalue of the adjacency matrix  $A_G$  of  $G$ . Then we have*

$$g_1(G) \leq \widehat{g}(G) := \begin{cases} \frac{n^2\lambda_2^2}{(\lambda_2+r)^2} & \text{if } r \leq 3\lambda_2, \\ \frac{n^2\lambda_2}{8(r-\lambda_2)} & \text{otherwise,} \end{cases} \quad \text{and} \quad h_1(G) \leq \widehat{h}(G) := \frac{n\lambda_2}{2(\lambda_2+r)}.$$

Moreover, we have equality  $g_1(G) = \widehat{g}(G)$  if  $G$  is vertex- and edge-transitive, and equality  $h_1(G) = \widehat{h}(G)$  if  $G$  is edge-transitive.

Observe that the bound  $h(G) \leq \widehat{h}(G)$  sharpens the bound  $h(G) \leq \frac{n}{r}\lambda_2$  by Vallentin [Val20]. Moreover, one can check that  $\widehat{h}(G) \leq \frac{1}{2}\sqrt{\widehat{g}(G)}$ , which mirrors the inequalities  $h(G) \leq \frac{1}{2}\sqrt{g(G)}$  and  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$  (in Proposition 7.2). We will see in Section 7.5 several classes of graphs for which strict inequality  $\widehat{h}(G) < \frac{1}{2}\sqrt{\widehat{g}(G)}$  holds and, in Section 7.4, we will compare the parameter  $\widehat{h}(\cdot)$  with other eigenvalue bounds by Hoffman and by Haemers [Haem97, Haem01].

**Bounds for the balanced parameters.** As we have seen earlier, the parameter  $\alpha_{\text{bal}}(G)$ , asking for the maximum cardinality of a balanced independent set in  $G$ , arises naturally when considering the parameters  $h(\cdot)$  and  $g(\cdot)$ . An additional motivation comes from its relevance to product-free sets in groups and other applications as in [AYRP07, MRU87, RL88, Tah06, YWWY05]. The question thus arises of finding semidefinite and eigenvalue-based bounds for  $\alpha_{\text{bal}}(G)$  (and the related parameters  $h_{\text{bal}}(G)$  and  $g_{\text{bal}}(G)$ ) that improve on the bounds  $h_1(G)$  and  $\widehat{h}(G)$  designed for the general (not necessarily balanced) parameters. We investigate this question in detail in Section 7.6. We define semidefinite bounds  $\text{las}_{\text{bal},1}(G)$  and  $\vartheta_{\text{bal}}(G)$  for  $\alpha_{\text{bal}}(G)$ ,  $g_{\text{bal},1}(G)$  for  $g_{\text{bal}}(G)$ , and  $h_{\text{bal},1}(G)$  for  $h_{\text{bal}}(G)$ , and we show they satisfy  $\frac{1}{4}\text{las}_{\text{bal},1}(G) \leq \frac{1}{2}\sqrt{g_{\text{bal},1}(G)} \leq h_{\text{bal},1}(G) = \frac{1}{4}\vartheta_{\text{bal}}(G)$  (see Proposition 7.33). Interestingly, the “balanced versions” of the theta number may lead to different parameters, i.e.,  $\text{las}_{\text{bal},1}(G) < \vartheta_{\text{bal}}(G)$  may hold (see Example 7.34). On the other hand, we show that the closed-form values obtained by restricting

the optimization to symmetric solutions in each of these semidefinite bounds in fact recover (up to the correct transformation) the eigenvalue bound  $\widehat{h}(G)$  (see Proposition 7.37).

## 7.2. Complexity results

In this section we prove several complexity results. Recall that a *clique* in  $G$  is a set of pairwise adjacent vertices and  $\omega(G)$  denotes the maximum cardinality of a clique in  $G$ , so that  $\omega(G) = \alpha(\overline{G})$ . We consider the following problems.

**PROBLEM 1 ( $\alpha$ -BAL-BIP).** *Given a bipartite graph  $G$ , decide whether  $\alpha(G) = \alpha_{\text{bal}}(G)$ , i.e., whether  $G$  has a balanced maximum independent set.*

**PROBLEM 2 (HALF-SIZE-CLIQUE-EDGE).** *Given a graph  $G = (V, E)$  with  $|V|$  even and  $|E| = \frac{1}{4}|V|(|V| - 2)$ , decide whether  $\omega(G) \geq \frac{|V|}{2}$ .*

**PROBLEM 3 (HALF-SIZE-CLIQUE).** *Given a graph  $G = (V, E)$  with  $|V|$  even, decide whether  $\omega(G) \geq \frac{|V|}{2}$ .*

**PROBLEM 4 (CLIQUE).** *Given a graph  $G$  and an integer  $k \in \mathbb{N}$ , decide whether  $\omega(G) \geq k$ .*

It is well-known that CLIQUE is an NP-complete problem [Kar72] as well as problem HALF-SIZE-CLIQUE; we refer, e.g., to [ADLRY94] for an easy reduction of CLIQUE to HALF-SIZE-CLIQUE. In what follows we will show the following reductions

$$\text{HALF-SIZE-CLIQUE} \leq_P \text{HALF-SIZE-CLIQUE-EDGE} \leq_P \alpha\text{-BAL-BIP}. \quad (7.10)$$

Here we say that  $L_1 \leq_P L_2$  if we have a polynomial-time algorithm permitting to encode an instance of  $L_1$  as an instance of  $L_2$ . We will show the first reduction in Theorem 7.7 and the second one in Theorem 7.11 below. Then, using the reductions in (7.10), we obtain the following complexity results.

**Theorem 7.4.** *Problem 1 ( $\alpha$ -BAL-BIP) is an NP-complete problem.*

**Corollary 7.5.** *Computing the parameter  $h(G)$  for  $G$  bipartite is NP-hard.*

**PROOF.** Recall that computing  $\alpha(G)$  in bipartite graphs can be done in polynomial time. Hence, if there is a polynomial time algorithm for computing  $h(G)$ , then one can decide in polynomial time whether  $h(G) = \frac{\alpha(G)}{4}$ , which is equivalent to Problem 1, in view of Lemma 7.1.  $\square$

The proof technique used to show the reduction from problem HALF-SIZE-CLIQUE-EDGE to problem  $\alpha$ -BAL-BIP will in fact allow to show a broader set of results. Namely it permits to show hardness of testing whether any of the following equalities holds:  $g(G) = g_{\text{bal}}(G)$ ,  $h(G) = h_{\text{bal}}(G)$ , or  $h(G) = \frac{1}{2}\sqrt{g(G)}$ . In other words, it is NP-hard to check whether any of the inequalities

in relation (7.3) holds at equality. See Corollary 7.12 below for these and other hardness results.

In the rest of the section we will prove the two reductions from relation (7.10) and related hardness results for the other (balanced) parameters. For this we use as a first ingredient the following graph constructions.

**Definition 7.6.** *Let  $G = (V(G), E(G))$  and  $H = (V(H), E(H))$  be two graphs with disjoint vertex sets and let  $k \geq 1$  be an integer.*

- (i) *The disjoint union of  $G$  and  $H$ , denoted by  $G \oplus H$ , is the graph with vertex set  $V(G) \cup V(H)$  and edge set  $E(G) \cup E(H)$ .*
- (ii) *The join of  $G$  and  $H$ , denoted by  $G \bowtie H$ , is the graph with vertex set  $V(G) \cup V(H)$  and edge set  $E(G) \cup E(H) \cup (V(G) \times V(H))$ .*
- (iii) *The  $k$ -th expansion of  $G$ , denoted by  $G^{(k)}$ , is the graph constructed as follows: its vertex set is  $\bigcup_{v \in V(G)} X_v$ , where  $X_v$  are disjoint sets, each of size  $k$ , and we have a clique on each  $X_v$  and a complete bipartite graph between  $X_u$  and  $X_v$  whenever  $\{u, v\} \in E(G)$ .*

Clearly we have the following relations:

$$|V(G \oplus H)| = |V(G)| + |V(H)|, \quad |E(G \oplus H)| = |E(G)| + |E(H)|, \quad (7.11)$$

$$\omega(G \oplus H) = \max\{\omega(G), \omega(H)\}, \quad (7.12)$$

$$|V(G \bowtie H)| = |V(G)| + |V(H)|, \quad (7.13)$$

$$|E(G \bowtie H)| = |E(G)| + |E(H)| + |V(G)| \cdot |V(H)|, \quad (7.14)$$

$$\omega(G \bowtie H) = \omega(G) + \omega(H), \quad (7.15)$$

$$|V(G^{(k)})| = k|V(G)|, \quad |E(G^{(k)})| = \binom{k}{2}|V(G)| + k^2|E(G)|, \quad (7.16)$$

$$\omega(G^{(k)}) = k\omega(G). \quad (7.17)$$

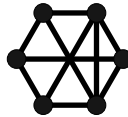


FIGURE 7.1. Graph  $F$ ,  $\omega(F) = 3$ , 6 nodes, 10 edges.

**Theorem 7.7.** HALF-SIZE-CLIQUE  $\leq_P$  HALF-SIZE-CLIQUE-EDGE.

PROOF. Let  $G$  be an instance of HALF-SIZE-CLIQUE, set  $|V(G)| = 2n$ ,  $|E(G)| = m$ . Let  $t$  be the smallest integer such that  $\binom{t}{2} \geq 9n^2 + n + m$ . Consider the graph  $F$  from Fig. 7.1 and define the graph

$$H := ((G \bowtie F^{(n)}) \bowtie K_t) \oplus H_0,$$

where  $H_0$  is a graph with  $t$  nodes and  $\binom{t}{2} - (9n^2 + n + m)$  edges. So the role of  $H_0$  is to add enough edges in order to ensure that  $|E(H)| = |V(H)|(|V(H)| - 2)/4$ .

Observe that  $H$  can be constructed in polynomial time. Using (7.11)-(7.17), we obtain

$$\begin{aligned} |V(H)| &= 8n + 2t, \\ |E(H)| &= (m + 6\binom{n}{2} + 10n^2 + 12n^2) + \binom{t}{2} + 8nt + \left(\binom{t}{2} - 9n^2 - n - m\right) \\ &= (4n + t)(4n + t - 1) = \frac{1}{4}(8n + 2t)(8n + 2t - 2), \\ \omega(H) &= \omega(G) + 3n + t. \end{aligned}$$

Hence,  $H$  is an instance of HALF-SIZE-CLIQUE-EDGE and  $\omega(H) \geq |V(H)|/2$  if and only if  $\omega(G) \geq |V(G)|/2$ . Therefore, if there is a polynomial time algorithm for solving HALF-SIZE-CLIQUE-EDGE, then we can solve HALF-SIZE-CLIQUE in polynomial time.  $\square$

As a next step we show the reduction of HALF-SIZE-CLIQUE-EDGE to  $\alpha$ -BAL-BIP. Our proof is inspired from an argument in [CK03], where the authors consider minimum vertex covers in a bipartite graph restricted to have at least  $k_1$  vertices in one side of the bipartition and at least  $k_2$  vertices in the other side. In [CK03, Theorem 3.1] it is shown that deciding existence of such vertex covers is NP-complete by giving a reduction from CLIQUE. We adapt this reduction by suitably selecting the values of  $k_1$  and  $k_2$ , considering independent sets (complements of vertex covers) instead of vertex covers, and modifying the graph construction used in [CK03].

The following graph construction will play a central role for the reduction of HALF-SIZE-CLIQUE-EDGE to  $\alpha$ -BAL-BIP (and other related problems).

**Definition 7.8.** *Given a graph  $G = (V, E)$  with  $n := |V|$  and  $m := |E|$ , consider the bipartite graph  $H_G = (V_1 \cup V_2, E_H)$  constructed as follows.*

- (i) *For each vertex  $v \in V$  we construct two vertices  $v_1 \in V_1$  and  $v_2 \in V_2$  and add the edge  $\{v_1, v_2\}$  to  $E_H$ .*
- (ii) *For each edge  $e \in E$  we construct two vertex sets  $L_e \subseteq V_1$  and  $R_e \subseteq V_2$  with  $|L_e| = |R_e| = n + 1$  and add all edges in  $L_e \times R_e$  to  $E_H$ .*
- (iii) *If  $v \in V$  is incident to  $e \in E$ , then we let  $v_1$  be adjacent in  $H_G$  to all vertices of  $R_e$ .*

Hence, setting  $L_V := \{v_1 : v \in V\}$ ,  $R_V := \{v_2 : v \in V\}$ ,  $L_E := \bigcup_{e \in E} L_e$ , and  $R_E := \bigcup_{e \in E} R_e$ , we have  $V_1 = L_V \cup L_E$  and  $V_2 = R_V \cup R_E$ , there is a perfect matching between  $L_V$  and  $R_V$ , there is a complete bipartite graph between  $L_e$  and  $R_e$  for each  $e \in E$ , and there is a complete bipartite graph between  $v_1 \in V_1$  and  $R_e$  for each edge  $e \in E$  containing  $v \in V$ .

The next lemma shows that the maximal independent sets in the bipartite graph  $H_G$  have a very special structure, which will be useful for the proof of Theorem 7.11 below.

**Lemma 7.9.** *Let  $G = (V, E)$  be a graph,  $n := |V|$ ,  $m := |E|$ , and let  $H_G$  be the associated bipartite graph as in Definition 7.8. Assume  $I \subseteq V(H_G) = V_1 \cup V_2$*

is a maximal independent set of  $H_G$ . Then  $I$  takes the following form

$$I \cap V_1 = \{v_1 : v \in A\} \cup \bigcup_{e \in E_1} L_e, \quad I \cap V_2 = \{v_2 : v \in B\} \cup \bigcup_{e \in E_2} R_e, \quad (7.18)$$

where  $A \subseteq V$ ,  $B = V \setminus A$ ,  $E_1$  is the set of edges  $e \in E$  that are incident to some node  $v \in A$ , and  $E_2 = E \setminus E_1$  (thus the set of edges  $e \in E$  contained in  $B$ ). Moreover,  $I$  is a maximum independent set of  $H_G$  and  $\alpha(H_G) = n + m(n + 1)$ . Conversely, any set  $I$  as in (7.18) is a (maximum) independent set of  $H_G$ .

PROOF. Assume  $I \subseteq V_1 \cup V_2$  is a maximal independent set of  $H_G$ . Set  $A := \{v \in V : v_1 \in I\}$ ,  $B := \{v \in V : v_2 \in I\}$ , and  $E_2 := E \setminus E_1$ , where  $E_1$  is the set of edges  $e \in E$  that are incident to some node  $v \in A$ ; we show that (7.18) holds. First, we have  $A \cap B = \emptyset$  (for, if  $v \in A \cap B$ , then the edge  $\{v_1, v_2\}$  of  $H_G$  would be contained in  $I$ , contradicting that  $I$  is independent). Moreover,  $A \cup B = V$  (for, if  $v \in V \setminus (A \cup B)$ , then the set  $I \cup \{v_2\}$  would be independent in  $H_G$ , contradicting the maximality of  $I$ ). So we have  $I \cap L_V = \{v_1 : v \in A\}$  and  $I \cap R_V = \{v_2 : v \in B\}$ . We now claim that  $I \cap L_E = \bigcup_{e \in E_1} L_e$  and  $I \cap R_E = \bigcup_{e \in E_1} R_e$ . First note that, if  $I \cap R_e \neq \emptyset$ , then  $e$  is not incident to any node of  $A$  and thus  $e \in E_2$ . Moreover, by maximality of  $I$ , we have  $R_e \subseteq I$  for any  $e \in E_2$ . So we indeed have  $I \cap R_E = \bigcup_{e \in E_2} R_e$  and in turn this implies  $I \cap L_E = \bigcup_{e \in E_1} L_e$ . Therefore we have  $|I| = n + m(n + 1)$ , which implies that  $\alpha(H_G) = n + m(n + 1)$  and that  $I$  is maximum independent. This concludes the proof (since the last (reverse) claim is straightforward to check).  $\square$

**Corollary 7.10.** *Let  $G = (V, E)$  be a graph and let  $H_G$  be the bipartite graph as in Definition 7.8. The following assertions are equivalent.*

- (i)  $\alpha_{\text{bal}}(H_G) = \alpha(H_G)$ .
- (ii)  $g_{\text{bal}}(H_G) = g(H_G)$ .
- (iii)  $h_{\text{bal}}(H_G) = h(H_G)$ .

PROOF. The implications (i)  $\implies$  (ii) and (i)  $\implies$  (iii) follow from relation (7.3). Conversely, assume (ii) holds and let  $(A, B)$  be a balanced optimal solution for  $g(H_G)$ . Then  $A \cup B$  is maximal independent in  $H_G$  and thus, by Lemma 7.9, it is maximum, so that  $\alpha(H_G) = |A \cup B| = \alpha_{\text{bal}}(H_G)$  as  $(A, B)$  is balanced. The same argument shows the implication (iii)  $\implies$  (i).  $\square$

Now we show the main result of the section, which combined with Theorem 7.7, implies Theorem 7.4.

**Theorem 7.11.** *Let  $G = (V, E)$  be a graph satisfying  $|E| = \frac{1}{4}|V|(|V| - 2)$  and let  $H_G$  be the associated bipartite graph as in Definition 7.8. The following assertions are equivalent.*

- (i)  $G$  has a clique of size  $|V|/2$ , i.e.,  $\omega(G) \geq |V|/2$ .
- (ii)  $\alpha(H_G) = \alpha_{\text{bal}}(H_G)$ .

Therefore, HALF-SIZE-CLIQUE-EDGE  $\leq_P$   $\alpha$ -BAL-BIP.

PROOF. We first show (i)  $\implies$  (ii). Assume  $C$  is a clique of  $G$  with  $|C| = |V|/2$ . Let  $E_2$  be the set of edges of  $G$  that are contained in  $C$ , so that  $E_1 := E \setminus E_2$  is the set of edges of  $G$  that are incident to some node in  $V \setminus C$ . By the assumption on  $G$  we have  $\binom{|V|/2}{2} = \frac{|E|}{2}$  and thus  $|E_2| = \binom{|V|/2}{2} = \frac{|E|}{2} = |E_1|$ . Consider the subset  $I \subseteq V_1 \cup V_2$  of  $V(H_G)$ , which is defined by

$$I \cap V_1 = \{v_1 : v \notin C\} \cup \bigcup_{e \in E_1} L_e, \quad I \cap V_2 = \{v_2 : v \in C\} \cup \bigcup_{e \in E_2} R_e.$$

By Lemma 7.9,  $I$  is a maximum independent set in  $H_G$  and  $\alpha(H_G) = n+m(n+1)$ . Moreover, we have  $|I \cap V_1| = |I \cap V_2|$ , which shows that  $\alpha_{\text{bal}}(H_G) = \alpha(H_G)$ .

Now we show (ii)  $\implies$  (i). By the assumption (ii),  $H_G$  has a balanced maximum independent set  $I$ . By Lemma 7.9,  $I$  takes the form as in (7.18). As  $I$  is balanced we have  $|I \cap V_1| = |I \cap V_2|$  and thus  $||A| - |B|| = (n+1)||E_2| - |E_1||$ . If  $|E_1| \neq |E_2|$  then the left hand side is at most  $n$  while the right hand side is at least  $n+1$ . Therefore we have  $|E_1| = |E_2| = |E|/2$  and  $|A| = |B| = |V|/2$ . Moreover,  $|E_2| \leq \binom{|B|}{2} = \binom{|V|/2}{2}$  since  $E_2$  consists of the edges that are contained in  $B$ . This gives  $|E| = 2|E_2| \leq 2\binom{|V|/2}{2} = |V|(|V|-2)/4$ . We now use the assumption  $|E| = |V|(|V|-2)/4$  on the number of edges of  $G$ , which implies that equality holds throughout and thus that  $B$  is a clique in  $G$  of size  $|B| = |V|/2$ , showing (i).  $\square$

**Corollary 7.12.** *Given a bipartite graph  $G$  it is NP-hard to decide whether any of the following equalities holds.*

- (i)  $g(G) = g_{\text{bal}}(G)$ .
- (ii)  $h(G) = h_{\text{bal}}(G)$ .
- (iii)  $h(G) = \frac{1}{4}\alpha(G)$ .
- (iv)  $\frac{1}{2}\sqrt{g(G)} = \frac{1}{4}\alpha(G)$ .
- (v)  $h(G) = \frac{1}{2}\sqrt{g(G)}$ .

PROOF. We show that it is NP-hard to check any of the equalities (i)-(v) for the class of bipartite graphs that are of the form  $H_G$  (as in Definition 7.8) for some graph  $G$  with  $|E| = \frac{1}{4}|V|(|V|-2)$ . The key fact is that, for bipartite graphs of the form  $H_G$ , any of the assertions (i)-(v) is equivalent to  $\alpha(H_G) = \alpha_{\text{bal}}(H_G)$ ; this was shown in Corollary 7.10 for (i)-(ii) and in relation (7.4) for (iii)-(iv), and one can easily verify that (v) implies (i). Then the corollary follows using Theorems 7.7 and 7.11 together with hardness of HALF-SIZE-CLIQUE.  $\square$

**Remark 7.13.** *The hardness results in Corollary 7.12 hold in fact for a broader class of bipartite graph parameters. For this consider a bivariate function  $f : \mathbb{R}_+^2 \rightarrow \mathbb{R}$  that satisfies the condition*

$$f(a, b) \leq \frac{a+b}{4}, \quad \text{and} \quad f(a, b) = \frac{a+b}{4} \iff a = b, \quad \text{for all } a, b \in \mathbb{N} \quad (7.19)$$

and define the corresponding graph parameter for a bipartite graph  $G$ .

$$f(G) := \max\{f(|A|, |B|) : (A, B) \text{ is bipartite biindependent in } G\}$$

Using relation (7.19) one can check the inequalities  $\frac{\alpha_{\text{bal}}(G)}{4} \leq f(G) \leq \frac{\alpha(G)}{4}$  and the equivalence  $f(G) = \frac{\alpha(G)}{4} \iff \alpha(G) = \alpha_{\text{bal}}(G)$ . Using Theorem 7.11, it follows that computing  $f(\cdot)$  is NP-hard (already for the bipartite graphs of the form  $H_G$  for some graph  $G$  with  $|V|(|V| - 2)/4$  edges).

Examples of functions satisfying (7.19) include  $f(a, b) = \frac{ab}{a+b}$  (giving the parameter  $h(G)$ ) and  $f(a, b) = \frac{1}{2}\sqrt{ab}$  (giving  $\frac{1}{2}\sqrt{g(G)}$ ), or any  $f(\cdot)$  nested between  $h(\cdot)$  and  $\frac{1}{2}\sqrt{g(\cdot)}$ . As another example, consider

$$f(a, b) := \left(\frac{1}{2}\sqrt{ab}\right)^p \left(\frac{a+b}{4}\right)^{1-p}$$

with  $0 \leq p \leq 1$ , which gives a graph parameter  $f(\cdot)$  nested between  $\frac{1}{2}\sqrt{g(\cdot)}$  and  $\frac{\alpha(\cdot)}{4}$ .

### 7.3. Semidefinite approximations for the parameters $g(G)$ and $h(G)$

In this section, we introduce semidefinite approximations for the parameters  $g(\cdot)$  and  $h(\cdot)$  from (7.1) and (7.2), which are both NP-hard to compute as we saw in the previous sections. Our approach relies on formulating the parameters  $g(\cdot)$  and  $h(\cdot)$  as 0-1 polynomial optimization problems and considering the corresponding Lasserre sum-of-squares hierarchies. This technique is the analog to the one described in Section 3.2.1 in Chapter 3 for approximating  $\alpha(G)$  in arbitrary graphs. We recall this formulation. Given a graph  $G$ , its stability number  $\alpha(G)$  can be formulated as follows:

$$\alpha(G) = \max \left\{ \sum_{i=1}^n x_i : x_i x_j = 0 \text{ for } \{i, j\} \in E, x_i^2 - x_i = 0 \text{ for } i \in V \right\},$$

and its corresponding Lasserre sum-of-squares hierarchy, already introduced in (3.7), reads

$$\text{las}_r(G) = \max \left\{ \lambda : \lambda - \sum_{i=1}^n x_i \in \Sigma_{2r} + I_{2r, G} \right\}.$$

As mentioned in Chapter 1, the parameter  $\text{las}_r(G)$  can be expressed via a semidefinite program and we have  $\alpha(G) \leq \text{las}_{r+1}(G) \leq \text{las}_r(G)$ , with equality  $\alpha(G) = \text{las}_r(G)$  if  $r \geq \alpha(G)$  [Lau03] (see Theorem 3.2). This last claim follows from the following fact shown in relation (3.8) (see also [Las01a] and [Lau03]). At order  $r = 1$  we obtain the bound  $\text{las}_1(G)$  which, after applying



SDP duality, can be checked to take the form

$$\text{las}_1(G) = \max \left\{ \langle I, X \rangle : X \in \mathcal{S}^n, \begin{pmatrix} 1 & \text{diag}(X)^\top \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, \right. \\ \left. X_{ij} = 0 \text{ for } \{i, j\} \in E \right\}, \quad (7.20)$$

which is a well-known formulation for  $\vartheta(G)$ , so that  $\text{las}_1(G) = \vartheta(G)$  (as already mentioned in Chapter 3).

Assume now  $G = (V = V_1 \cup V_2, E)$  is a bipartite graph. Define the matrix

$$C := \frac{1}{2} \begin{pmatrix} 0 & J_{|V_1|, |V_2|} \\ J_{|V_2|, |V_1|} & 0 \end{pmatrix} \in \mathcal{S}^{|V|}, \quad (7.21)$$

so that  $x^\top C x = (\sum_{i \in V_1} x_i)(\sum_{j \in V_2} x_j)$ . Observe that one can encode a biindependent pair  $(A, B)$  with  $A \subseteq V_1$  and  $B \subseteq V_2$  by its characteristic vector  $x = \chi^{A \cup B}$ . Then we can express the parameters  $g(G)$  and  $h(G)$  as

$$g(G) = \max \left\{ x^\top C x : x_i^2 = x_i \ (i \in V), \ x_i x_j = 0 \ (\{i, j\} \in E) \right\}, \quad (7.22)$$

$$h(G) = \max \left\{ \frac{x^\top C x}{x^\top x} : x_i^2 = x_i \ (i \in V), \ x_i x_j = 0 \ (\{i, j\} \in E) \right\}. \quad (7.23)$$

The Lasserre bounds of order  $r$  for  $g(G)$  and  $h(G)$  read, respectively,

$$g_r(G) := \min \{ \lambda : \lambda - x^\top C x \in \Sigma_{2r} + I_{G, 2r} \}, \quad (7.24)$$

$$h_r(G) := \min \{ \lambda : x^\top (\lambda I - C) x \in \Sigma_{2r} + I_{G, 2r} \}, \quad (7.25)$$

and the next result follows as a direct application of relation (3.8).

**Lemma 7.14.** *Let  $G$  be a bipartite graph. For any integer  $r \geq 1$ , we have  $g(G) \leq g_r(G)$  and  $h(G) \leq h_r(G)$ , with equality if  $r \geq \alpha(G)$ .*

**7.3.1. Semidefinite formulations for the Lasserre bounds  $h_1(G)$  and  $g_1(G)$ .** In this section we give explicit semidefinite formulations for the Lasserre bounds (7.24) and (7.25) of order  $r = 1$  for  $g(G)$  and  $h(G)$ . In particular, we indicate how to obtain the formulations given earlier in (7.8) and (7.9). Recall that  $\mathcal{S}_G$  consists of the matrices in  $\mathcal{S}^{|V|}$  that are supported by  $G$ . We begin with a claim expressing polynomials in the truncated ideal  $I_{G,2}$  that we will repeatedly use.

**Lemma 7.15.** *Given a graph  $G = (V, E)$  and a matrix  $M \in \mathcal{S}^{1+|V|}$  (indexed by  $\{0\} \cup V$ ), we have  $[x]_1^\top M[x]_1 \in I_{G,2}$  if and only if  $M$  takes the form*

$$M = \begin{pmatrix} 0 & -u^\top/2 \\ -u/2 & \text{Diag}(u) + Z \end{pmatrix} \text{ for some } u \in \mathbb{R}^{|V|}, \ Z \in \mathcal{S}_G. \quad (7.26)$$

PROOF. By definition,  $[x]_1^\top M[x]_1 \in I_{G,2}$  if

$$[x]_1^\top M[x]_1 = \sum_{i \in V} u_i (x_i^2 - x_i) + \sum_{\{i,j\} \in E} u_{ij} x_i x_j$$

for some  $u_i, u_{ij} \in \mathbb{R}$ . The result follows by equating coefficients at both sides of this polynomial identity.  $\square$

We now give semidefinite formulations for the parameters  $h_1(G)$  and  $g_1(G)$ .

**Lemma 7.16.** *Let  $G = (V = V_1 \cup V_2, E)$  be a bipartite graph. Then the Lasserre bound of order  $r = 1$  for  $h(G)$  can be reformulated as*

$$h_1(G) = \min_{\lambda \in \mathbb{R}, Z \in \mathcal{S}^V} \{ \lambda : \lambda I + Z - C \succeq 0, Z \in \mathcal{S}_G \}, \quad (7.27)$$

$$= \max_{X \in \mathcal{S}^V} \{ \langle C, X \rangle : X \succeq 0, \text{Tr}(X) = 1, X_{ij} = 0 \text{ for } \{i, j\} \in E \}. \quad (7.28)$$

PROOF. By definition,  $h_1(G)$  is the smallest scalar  $\lambda$  for which we have  $x^\top(\lambda I - C)x \in \Sigma_2 + I_{G,2}$ , i.e., the smallest  $\lambda$  for which  $[x]_1^\top Q[x]_1 - x^\top(\lambda I - C)x$  belongs to  $I_{G,2}$  for some matrix  $Q \succeq 0$  (indexed by  $\{0\} \cup V$ ). Using Lemma 7.15 we obtain that  $Q_{00} = 0$  and thus  $Q_{0i} = 0$  for all  $i \in V$  (as  $Q \succeq 0$ ). From this follows that the principal submatrix indexed by  $V$  takes the form  $Q[V] = Z + \lambda I - C$  for some  $Z \in \mathcal{S}_G$  and we arrive at the formulation (7.27) for  $h_1(G)$ . By taking the semidefinite dual we obtain the formulation (7.28). Observe that strong duality holds because program (7.28) is feasible with  $X = \frac{1}{n}I$  and program (7.27) is clearly strictly feasible for some  $\lambda \gg 0$ .  $\square$

**Lemma 7.17.** *Let  $G$  be a bipartite graph. Then we have*

$$g_1(G) = \min_{\lambda \in \mathbb{R}, u \in \mathbb{R}^V, Z \in \mathcal{S}^V} \left\{ \lambda : \begin{pmatrix} \lambda & u^\top/2 \\ u/2 & \text{Diag}(u) - C + Z \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}, \quad (7.29)$$

$$= \max_{X \in \mathcal{S}^V} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^\top \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, X_{ij} = 0 \text{ for } \{i, j\} \in E \right\}. \quad (7.30)$$

PROOF. By definition  $g_1(G)$  is the smallest scalar  $\lambda$  for which we have  $\lambda - x^\top Cx \in \Sigma_2 + I_{G,2}$ . In other words this is the smallest  $\lambda$  for which there exists  $Q \succeq 0$  such that  $[x]_1^\top (Q - \begin{pmatrix} \lambda & 0 \\ 0 & -C \end{pmatrix}) [x]_1 \in I_{G,2}$ . Using Lemma 7.15, we obtain the formulation of  $g_1(G)$  as in (7.29). Then the formulation (7.30) follows by taking the dual of the semidefinite program (7.29). Observe that strong duality holds as program (7.30) is feasible and program (7.29) is strictly feasible for  $Z = 0$  and suitable  $\lambda$  and  $u$ .  $\square$

**Remark 7.18.** *In order to highlight some similarities and differences between the parameters  $\text{las}_1(G)$ ,  $g_1(G)$  and  $h_1(G)$ , we indicate how to derive the formulation (7.20) of  $\text{las}_1(G)$ . Let us start with the definition of  $\text{las}_1(G)$  as the smallest  $\lambda$  for which  $\lambda - \sum_{i \in V} x_i \in \Sigma_2 + I_{G,2}$ . Since  $\sum_{i \in V} x_i - x^\top Ix \in I_{G,2}$  we can alternatively search for the smallest  $\lambda$  for which*

$$[x]_1^\top (Q - \begin{pmatrix} \lambda & 0 \\ 0 & -I \end{pmatrix}) [x]_1 \in I_{G,2}.$$

Using Lemma 7.15, we obtain

$$\text{las}_1(G) = \min_{\lambda \in \mathbb{R}, u \in \mathbb{R}^V, Z \in \mathcal{S}^V} \left\{ \lambda : \begin{pmatrix} \lambda & u^\top/2 \\ u/2 & \text{Diag}(u) - I + Z \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}. \tag{7.31}$$

Taking the dual semidefinite program of (7.31), we obtain the formulation (7.20).

Note the similarity between programs (7.29) and (7.31), which are the same up to exchanging the matrices  $C$  and  $I$ . Note also that it is possible to simplify program (7.31) and to bring it in the form

$$\text{las}_1(G) = \min_{\lambda \in \mathbb{R}, Z \in \mathcal{S}^V} \left\{ \lambda : \begin{pmatrix} \lambda & e^\top \\ e & I + Z \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}, \tag{7.32}$$

which is another well-known formulation of  $\vartheta(G)$ . To see this, call  $Q$  the matrix in program (7.31). As  $Q_{ii} = u_i - 1 \geq 0$  we have  $u_i \geq 1$  for all  $i \in V$ . By scaling the  $i$ th column/row of  $Q$  by  $2/u_i$  and adding  $1 - \frac{4}{u_i^2}(u_i - 1) = \frac{(u_i - 2)^2}{u_i^2} \geq 0$  to entry  $Q_{ii}$ , we obtain a new matrix  $Q' \succeq 0$  satisfying  $Q'_{0i} = Q'_{ii} = 1$  for all  $i \in V$ , thus feasible for (7.32). This shows the equivalence of (7.31) and (7.32).

Note, however, that the above rescaling trick could not be applied to program (7.29); indeed if  $Q$  denotes the matrix appearing in (7.29), then one must have  $Q_{ij} = -1/2$  for all positions  $(i, j) \in V_1 \times V_2$  corresponding to non-edges of  $G$ .

**7.3.2. Comparison of the Lasserre bounds  $h_1(G)$  and  $g_1(G)$ .** In this section, we show the following inequalities for any bipartite graph  $G$ :

$$h(G) \leq \frac{1}{2}\sqrt{g(G)} \leq h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)} \leq \frac{1}{4}\alpha(G),$$

that were claimed in Proposition 7.2. One may have the strict inequalities  $h_1(G) < \frac{1}{2}\sqrt{g_1(G)} < \frac{1}{4}\alpha(G)$ , e.g., when  $G$  is the complete bipartite graph  $K_{n,n}$  minus a perfect matching and  $n \geq 5$  (see Section 7.5.2). Recall that we already know  $h(G) \leq \frac{1}{2}\sqrt{g(G)}$  from Lemma 7.1. Hence, in order to show Proposition 7.2, it suffices to show that the inequalities  $\frac{1}{2}\sqrt{g(G)} \leq h_1(G)$ ,  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$ ,  $h_1(G) \leq \frac{1}{4}\alpha(G)$ , and  $g_1(G) \leq \alpha(G)h_1(G)$  hold.

**Proof of  $\frac{1}{2}\sqrt{g(G)} \leq h_1(G)$ .** Let  $(A, B)$  be an optimal solution for  $g(G)$  with  $|A| =: a, |B| =: b$  and let  $(\lambda, Z)$  be a feasible solution for the formulation (7.27) of  $h_1(G)$ ; we show that  $\lambda \geq \frac{1}{2}\sqrt{ab}$ . By assumption, we have that the matrix  $M := \lambda I + Z - C$  is positive semidefinite and thus also its principal submatrix  $M[A \cup B]$  is positive semidefinite. Observe that  $M[A \cup B]$  has the block-form

$$M[A \cup B] = \begin{pmatrix} \lambda I_a & -\frac{1}{2}J_{a,b} \\ -\frac{1}{2}J_{b,a} & \lambda I_b \end{pmatrix},$$

because  $Z_{ij} = 0$  for  $i \in A, j \in B$  as  $A \cup B$  is independent. By taking a Schur complement we obtain that  $M[A \cup B] \succeq 0$  if and only if  $\lambda I_a - \frac{b}{4\lambda}J_{a,a} \succeq 0$ . This

implies  $\lambda \geq \frac{1}{2}\sqrt{ab} = \frac{1}{2}\sqrt{g(G)}$  and thus  $h_1(G) \geq \frac{1}{2}\sqrt{g(G)}$ .  $\square$

**Proof of  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$ .** Let  $X$  be an optimal solution for the formulation (7.28) of  $h_1(G)$ . Then  $X \succeq 0$  and thus  $X = (y_i^\top y_j)_{i,j \in V}$  for some vectors  $y_i \in \mathbb{R}^{|V|}$  ( $i \in V$ ). We may assume without loss of generality that  $y_i \neq 0$  for  $i \in V$  (since, if  $y_i = 0$ , then we just replace  $X$  by its principal submatrix indexed by  $V \setminus \{i\}$ ). Define the vectors  $y' := \sum_{i \in V_1} y_i$  and  $y'' := \sum_{i \in V_2} y_i$ , so that  $h_1(G) = \langle C, X \rangle = (y')^\top y''$ . To shorten notation we set  $h := h_1(G) = (y')^\top y''$ . We may assume  $h > 0$ , else there is nothing to prove. For  $\varepsilon = \pm 1$ , define the vector  $d_\varepsilon := \frac{y' + \varepsilon y''}{\|y' + \varepsilon y''\|}$ . Here the convention is that we consider the vector  $d_\varepsilon$  only if  $y' + \varepsilon y'' \neq 0$ . Note that at least one of  $d_1$  and  $d_{-1}$  is well-defined (since otherwise one would have  $y' = y'' = 0$ , implying  $h_1(G) = 0$ , a contradiction). Then let  $X_\varepsilon$  denote the Gram matrix of the vectors  $\frac{d_\varepsilon^\top y_i}{\|y_i\|^2} y_i$  for  $i \in V$ ; we claim that  $X_\varepsilon$  is feasible for the formulation (7.30) of  $g_1(G)$ . To see it, consider the matrix  $Y_\varepsilon$  defined as the Gram matrix of the vectors  $d_\varepsilon$  and  $\frac{d_\varepsilon^\top y_i}{\|y_i\|^2} y_i$  for  $i \in V$ , so that  $X_\varepsilon$  is its principal submatrix indexed by  $V$ , and note that  $Y_\varepsilon \succeq 0$ ,  $(Y_\varepsilon)_{00} = 1$ ,  $(Y_\varepsilon)_{0i} = (Y_\varepsilon)_{ii}$  for  $i \in V$ , and  $(Y_\varepsilon)_{ij} = 0$  if  $\{i, j\} \in E$ . Hence, if one can show that  $\langle C, X_\varepsilon \rangle \geq 4\langle C, X \rangle^2$  for some  $\varepsilon \in \{\pm 1\}$ , then this implies  $g_1(G) \geq \langle C, X_\varepsilon \rangle \geq 4\langle C, X \rangle^2 = 4h_1(G)^2$  and the proof is complete. The rest of the proof is devoted to showing that  $\langle C, X_\varepsilon \rangle \geq 4\langle C, X \rangle^2$  for some  $\varepsilon \in \{\pm 1\}$ , and is a bit technical.

In a first step, we show that the vectors  $y_i$  ( $i \in V$ ) satisfy the following relations

$$y_i^\top y'' = 2h \|y_i\|^2 \quad (i \in V_1), \quad (7.33)$$

$$y_j^\top y' = 2h \|y_j\|^2 \quad (j \in V_2). \quad (7.34)$$

For this consider an optimal solution  $S := hI + Z - C$  of the program (7.27) defining  $h_1(G)$ , where  $Z \in \mathcal{S}_G$ . As  $X$  and  $S$  are primal and dual optimal solutions we must have  $XS = 0$ , i.e.,  $0 = hX + XZ - XC$ . We now compute the diagonal entries. Note that  $(XZ)_{ii} = 0$  for all  $i \in V$  (since, for each  $k \in V$ , we have  $X_{ik} = 0$  or  $Z_{ki} = 0$ ). Hence, for  $i \in V_1$ , we have  $h\|y_i\|^2 = hX_{ii} = (XC)_{ii} = \frac{1}{2} \sum_{j \in V_2} X_{ij} = \frac{1}{2} y_i^\top y''$ , and, for  $j \in V_2$ , we have  $h\|y_j\|^2 = hX_{jj} = (XC)_{jj} = \frac{1}{2} \sum_{i \in V_1} X_{ij} = \frac{1}{2} y_j^\top y'$ . So (7.33) and (7.34) hold.

We now proceed to compute

$$\langle C, X_\varepsilon \rangle = \sum_{(i,j) \in V_1 \times V_2} \frac{d_\varepsilon^\top y_i \cdot d_\varepsilon^\top y_j}{\|y_i\|^2 \|y_j\|^2} \cdot y_i^\top y_j. \quad (7.35)$$

First, we compute (part of) the inner term for  $i \in V_1$  and  $j \in V_2$ :

$$\frac{d_\varepsilon^\top y_i \cdot d_\varepsilon^\top y_j}{\|y_i\|^2 \|y_j\|^2} = \frac{1}{\|y' + \varepsilon y''\|^2} \frac{(y' + \varepsilon y'')^\top y_i \cdot (y' + \varepsilon y'')^\top y_j}{\|y_i\|^2 \|y_j\|^2} \quad (7.36)$$

$$= \frac{1}{\|y' + \varepsilon y''\|^2} \left( 2h \frac{(y')^\top y_i}{\|y_i\|^2} + 2h \frac{(y'')^\top y_j}{\|y_j\|^2} + \varepsilon \frac{(y')^\top y_i \cdot (y'')^\top y_j}{\|y_i\|^2 \|y_j\|^2} + 4h^2 \varepsilon \right), \quad (7.37)$$

where we have used relations (7.33), (7.34) and that  $\varepsilon^2 = 1$  to carry out the simplifications. Next observe that

$$\sum_{(i,j) \in V_1 \times V_2} \frac{(y')^\top y_i}{\|y_i\|^2} y_i^\top y_j = \sum_{i \in V_1} \frac{(y')^\top y_i}{\|y_i\|^2} \left( \sum_{j \in V_2} y_i^\top y_j \right) \quad (7.38)$$

$$= \sum_{i \in V_1} \frac{(y')^\top y_i}{\|y_i\|^2} y_i^\top y'' = 2h \sum_{i \in V_1} (y')^\top y_i = 2h \|y'\|^2, \quad (7.39)$$

where we have used again relation (7.33). In the same way we have

$$\sum_{(i,j) \in V_1 \times V_2} \frac{(y'')^\top y_j}{\|y_j\|^2} y_i^\top y_j = 2h \|y''\|^2. \quad (7.40)$$

Combining (7.35), (7.37), (7.38) and (7.40), we obtain

$$\begin{aligned} \langle C, X_\varepsilon \rangle &= \frac{1}{\|y' + \varepsilon y''\|^2} \left( 4h^2 (\|y'\|^2 + \|y''\|^2 + \varepsilon (y')^\top y'') \right) \\ &\quad + \varepsilon \sum_{(i,j) \in V_1 \times V_2} \frac{(y')^\top y_i \cdot (y'')^\top y_j \cdot y_i^\top y_j}{\|y_i\|^2 \|y_j\|^2} \\ &= \frac{1}{\|y' + \varepsilon y''\|^2} \left( 4h^2 \|y' + \varepsilon y''\|^2 - 4h^2 \varepsilon (y')^\top y'' \right) \\ &\quad + \varepsilon \sum_{(i,j) \in V_1 \times V_2} \frac{(y')^\top y_i \cdot (y'')^\top y_j \cdot y_i^\top y_j}{\|y_i\|^2 \|y_j\|^2} \\ &= 4h^2 + \frac{\varepsilon}{\|y' + \varepsilon y''\|^2} \underbrace{\left( \sum_{(i,j) \in V_1 \times V_2} \frac{(y')^\top y_i \cdot (y'')^\top y_j \cdot y_i^\top y_j}{\|y_i\|^2 \|y_j\|^2} - 4h^3 \right)}_{=:\varphi} \\ &= 4h^2 + \frac{\varepsilon \cdot \varphi}{\|y' + \varepsilon y''\|^2}. \end{aligned}$$

We can now conclude the proof. Assume first  $y' \pm y'' \neq 0$ , so that both  $d_1$  and  $d_{-1}$  are well-defined. If  $\varphi \geq 0$  then  $\langle C, X_1 \rangle \geq 4h^2$ . Otherwise, if  $\varphi < 0$ , then  $\langle C, X_{-1} \rangle \geq 4h^2$ . So we have shown the desired result:  $\langle C, X_\varepsilon \rangle \geq 4h^2$  for some  $\varepsilon \in \{\pm 1\}$ . Consider now the case when  $y' = \varepsilon y''$  for some  $\varepsilon \in \{\pm 1\}$ . Then, using relations (7.33) and (7.34), we obtain that  $\varphi = 0$ . Hence, if  $y' = y''$

(resp.,  $y' = -y''$ ), then we have  $\langle C, X_1 \rangle \geq 4h^2$  (resp.,  $\langle C, X_{-1} \rangle \geq 4h^2$ ), which concludes the proof.  $\square$

**Remark 7.19.** Note that the proof for the inequality  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$  resembles - but is technically more involved than - the classical proof for the inequality  $\text{las}_1(G) \geq \vartheta(G)$ , where  $\text{las}_1(G)$  is given by (7.20) and  $\vartheta(G)$  by (3.1) and  $G$  is an arbitrary graph. (The reverse inequality  $\vartheta(G) \geq \text{las}_1(G)$  is straightforward.) We sketch the proof for  $\text{las}_1(G) \geq \vartheta(G)$  in order to highlight the resemblance with the proof above for  $\frac{1}{2}\sqrt{g_1(G)} \geq h_1(G)$ . So assume  $X$  is optimal for (3.1) (defined as the Gram matrix of vectors  $y_i$  for  $i \in V$ ) and construct the matrix  $X_1$  (as the Gram matrix of the vectors  $\frac{d_1^\top y_i}{\|y_i\|} y_i$  for  $i \in V$ , where  $d_1 := (\sum_{i \in V} y_i) / \|\sum_{i \in V} y_i\|$ ). Then,  $\vartheta(G) = \langle J, X \rangle = \|\sum_{i \in V} y_i\|^2$ ,  $1 = \langle I, X \rangle = \sum_{i \in V} \|y_i\|^2$ , and  $y_i^\top y_j = 0$  if  $\{i, j\} \in E$ . This implies  $X_1$  is feasible for (7.20), and thus  $\text{las}_1(G) \geq \langle X_1, I \rangle$ . It suffices now to check that  $\langle X_1, I \rangle = \sum_{i \in V} \frac{(d_1^\top y_i)^2}{\|y_i\|^2} \geq \|\sum_{i \in V} y_i\|^2 = \vartheta(G)$ . But this follows easily using Cauchy-Schwartz inequality, namely

$$\begin{aligned} \|\sum_{i \in V} y_i\|^2 &= (d_1^\top \sum_{i \in V} y_i)^2 = \left( \sum_{i \in V} \frac{d_1^\top y_i}{\|y_i\|} \|y_i\| \right)^2 \leq \left( \sum_{i \in V} \frac{(d_1^\top y_i)^2}{\|y_i\|^2} \right) \left( \sum_{i \in V} \|y_i\|^2 \right) \\ &= \sum_{i \in V} \frac{(d_1^\top y_i)^2}{\|y_i\|^2}. \end{aligned}$$

**Proof of  $h_1(G) \leq \frac{1}{4}\alpha(G)$ .** Let  $X$  be optimal for the formulation (7.28) of  $h_1(G)$ . Then  $X$  is feasible for (3.1) and thus  $\vartheta(G) \geq \langle J, X \rangle$ . Since  $J - 4C \succeq 0$  this implies  $\langle J, X \rangle \geq 4\langle C, X \rangle = 4h_1(G)$ . Combining both inequalities we get  $4h_1(G) \leq \vartheta(G) = \alpha(G)$ .  $\square$

**Proof of  $g_1(G) \leq \alpha(G)h_1(G)$ .** Let  $X$  be an optimal solution for the formulation (7.30) of  $g_1(G)$ . Then,  $\frac{X}{\text{Tr}(X)}$  is feasible for  $h_1(G)$  and thus we have  $g_1(G) = \langle C, X \rangle \leq h_1(G) \cdot \text{Tr}(X)$ . On the other hand,  $X$  is feasible for (7.20), which gives  $\vartheta(G) \geq \text{Tr}(X)$ . Combining these two facts we obtain that  $g_1(G) \leq h_1(G) \cdot \vartheta(G) = h_1(G) \cdot \alpha(G)$ .  $\square$

**Remark 7.20.** So we have the following chain of inequalities for any bipartite graph  $G$ ,

$$\frac{1}{4}\alpha_{\text{bal}}(G) \leq h(G) \leq \frac{1}{2}\sqrt{g(G)} \leq h_1(G) \leq \frac{1}{4}\alpha(G)$$

(Proposition 7.2 and Lemma 7.1). Hence, equality  $\alpha(G) = \alpha_{\text{bal}}(G)$  implies  $h_1(G) = h(G)$ . Observe that the reverse implication holds when restricting to the bipartite graphs of the form  $H_G$  (constructed from some graph  $G$  as in Definition 7.8). Indeed,  $h_1(H_G) = h(H_G)$  implies  $\frac{1}{2}\sqrt{g(H_G)} = h(H_G)$ , which in turn implies  $g(H_G) = g_{\text{bal}}(H_G)$  (Corollary 7.12 and its proof) and thus  $\alpha(H_G) = \alpha_{\text{bal}}(H_G)$  (Corollary 7.10). This shows that deciding whether

the parameter  $h(\cdot)$  coincides with its semidefinite relaxation  $h_1(\cdot)$  is an NP-hard problem (already when restricting to the bipartite graphs of the form  $H_G$ , recall Theorem 7.11). This can be seen as an analog of the hardness of deciding whether the basic semidefinite relaxation of the maximum cut problem is exact, as shown in [DP93].

#### 7.4. Eigenvalue bounds for the parameters $g(G)$ and $h(G)$

Let  $G = (V, E)$  be a bipartite graph, with adjacency matrix  $A_G$ . We have introduced in Lemmas 7.16 and 7.17 the parameters  $g_1(G)$  and  $h_1(G)$  that, respectively, upper bound the parameters  $g(G)$  and  $h(G)$ . For convenience, we repeat their formulations

$$g_1(G) = \min_{\lambda \in \mathbb{R}, Z \in \mathcal{S}^V, u \in \mathbb{R}^V} \left\{ \lambda : \lambda(\text{Diag}(u) - C + Z) - \frac{1}{4}uu^T \succeq 0, \lambda \geq 0, Z \in \mathcal{S}_G \right\},$$

$$h_1(G) = \min_{\lambda \in \mathbb{R}, Z \in \mathcal{S}^V} \left\{ \lambda : \lambda I + Z - C \succeq 0, Z \in \mathcal{S}_G \right\}$$

(where the formulation for  $g_1(G)$  follows from (7.29) after taking the Schur complement with respect to the upper left corner  $\lambda$ ). In order to obtain closed-form parameters, one restricts the optimization in each of the above programs to matrices  $Z = tA_G$  (for some  $t \in \mathbb{R}$ ) and, for the parameter  $g_1(G)$ , to vectors  $u = \mu e$  (for some  $\mu \in \mathbb{R}$ ). Let  $\hat{g}(G)$  and  $\hat{h}(G)$  denote the parameters obtained in this way, so that  $g_1(G) \leq \hat{g}(G)$  and  $h_1(G) \leq \hat{h}(G)$ . When the graph  $G$  is regular, the all-ones vector is an eigenvector of the matrices involved in the programs defining  $\hat{g}(G)$  and  $\hat{h}(G)$ , and, as we will show below, this allows to show the closed-form expressions claimed in Proposition 7.3 for  $\hat{g}(G)$  and  $\hat{h}(G)$  in terms of the second largest eigenvalue  $\lambda_2$  of  $A_G$  and  $n := |V_1| = |V_2|$ .

We will use the following basic result about the eigenvalues of  $A_G$ . We refer, e.g., to the book by Brouwer and Haemers [BH17] for general background about eigenvalues of graphs.

**Lemma 7.21.** *Assume  $G = (V_1 \cup V_2, E)$  is a bipartite  $r$ -regular graph with  $|V_1| = |V_2| =: n \geq 2$ . Then its adjacency matrix is of the form*

$$A_G = \begin{pmatrix} 0 & M_G \\ M_G^T & 0 \end{pmatrix}, \quad \text{where } M_G \in \mathbb{R}^{|V_1| \times |V_2|}, \quad (7.41)$$

the eigenvalues of  $A_G$  are  $\pm \sqrt{\lambda_i(M_G M_G^T)}$  for  $i \in [n]$ ,  $\lambda_1(A_G) = r$ ,  $\lambda_{2n}(A_G) = -r$ , and  $\lambda_2(A_G) \geq 0$ , with equality  $\lambda_2(A_G) = 0$  if and only if  $G$  is complete bipartite. In the case when  $G = B(H)$  is the bipartite double of an  $r$ -regular graph  $H$ , we have  $M_G = A_H$ , the eigenvalues of  $A_{B(H)}$  are  $\pm \lambda_i(A_H)$  for  $i \in [n]$  and thus  $\lambda_2(A_{B(H)}) = \max\{\lambda_2(A_H), -\lambda_n(A_H)\}$ . When  $G = B_0(H)$  is the extended bipartite double of  $H$ , we have  $M_G = A_H + I$  and  $\lambda_2(A_{B_0(H)}) = \max\{\lambda_2(A_H) + 1, -\lambda_n(A_H) - 1\}$ .

**7.4.1. An eigenvalue-based upper bound  $\widehat{h}(G)$  for  $h(G)$ .** We give a closed-form eigenvalue-based upper bound for the parameter  $h(G)$  in the case when the bipartite graph  $G$  is  $r$ -regular. Let  $n := |V_1| = |V_2|$  and let  $\lambda_2$  denote the second largest eigenvalue of  $A_G$  (i.e., the second largest singular value of  $M_G$ , by Lemma 7.21). Vallentin [Val20] shows that  $h(G) \leq \frac{n}{r}\lambda_2$ , our next result gives a sharpening of this bound.

**Proposition 7.22.** *Assume  $G$  is a bipartite  $r$ -regular graph, set  $|V_1| = |V_2| =: n$ , and let  $\lambda_2$  be the second largest eigenvalue of its adjacency matrix  $A_G$ . Then we have*

$$h_1(G) \leq \widehat{h}(G) = \frac{n}{2} \frac{\lambda_2}{r + \lambda_2} \leq \frac{n}{r} \lambda_2. \quad (7.42)$$

Moreover, equality  $h_1(G) = \frac{n}{2} \frac{\lambda_2}{r + \lambda_2}$  holds when  $G$  is edge-transitive.

PROOF. We may assume  $G$  is not complete bipartite (else  $\lambda_2 = 0$  and  $h(G) = h_1(G) = \widehat{h}(G) = 0$ ). The inequality  $\frac{n}{2} \frac{\lambda_2}{r + \lambda_2} \leq \frac{n}{2} \lambda_2$  is clear; we now show  $h_1(G) \leq \frac{n}{2} \frac{\lambda_2}{r + \lambda_2}$ . For this we use the formulation of  $h_1(G)$  from (7.27), where we restrict the optimization to matrices  $Z$  of the form  $Z = tA_G$  for some scalar  $t \in \mathbb{R}$ ; we will show that the resulting optimal value is equal to  $\frac{n}{2} \frac{\lambda_2}{r + \lambda_2}$ . Note that when  $G$  is edge-transitive this restriction can be made without loss of generality. Thus we aim to compute the optimum value of the program

$$\widehat{h}(G) := \min_{\lambda, t \in \mathbb{R}} \{ \lambda : \lambda I + tA_G - C \succeq 0 \}, \quad (7.43)$$

which upper bounds  $h_1(G)$  and is equal to it when  $G$  is edge-transitive. By taking a Schur complement, the matrix

$$\lambda I + tA_G - C = \begin{pmatrix} \lambda I & tM_G - \frac{1}{2}J \\ tM_G^\top - \frac{1}{2}J & \lambda I \end{pmatrix}$$

is positive semidefinite if and only if  $\lambda > 0$  and the matrix

$$\begin{aligned} \lambda^2 I - (tM_G - \frac{1}{2}J)(tM_G^\top - \frac{1}{2}J) &= \lambda^2 I - (t^2 M_G M_G^\top - \frac{t}{2} M_G J - \frac{t}{2} J M_G^\top + \frac{1}{4} J^2) \\ &= \lambda^2 I - t^2 M_G M_G^\top + \frac{rt}{2} J + \frac{rt}{2} J - \frac{n}{4} J \\ &= \lambda^2 I - t^2 M_G M_G^\top + (rt - \frac{n}{4}) J =: Q \end{aligned}$$

is positive semidefinite. Since  $G$  is not complete bipartite we have  $\lambda > 0$ . We now analyze when  $Q$  is positive semidefinite. The all-ones vector  $e$  is an eigenvector of  $M_G M_G^\top$  and  $J$ , and thus also of  $Q$ . Any eigenvector  $w \perp e$  of  $M_G M_G^\top$  for  $\lambda_i(M_G M_G^\top)$  ( $2 \leq i \leq n$ ) is an eigenvector of  $Q$ . Then the eigenvalues of  $Q$  at these eigenvectors are as follows:

$$\begin{aligned} \text{at } e: & \quad \lambda^2 - t^2 r^2 + n(tr - \frac{n}{4}), \\ \text{at } w \perp e: & \quad \lambda^2 - t^2 \lambda_i(M_G M_G^\top) \quad \text{for } i = 2, \dots, n. \end{aligned}$$



Hence,  $Q \succeq 0$  if and only if  $\lambda^2 - t^2r^2 + n(tr - \frac{n}{4}) \geq 0$  and  $\lambda^2 - t^2\lambda_i(M_G M_G^T) \geq 0$  for any  $i \geq 2$ , which is equivalent to  $\lambda^2 - t^2\lambda_2^2 \geq 0$  (recall Lemma 7.21). Therefore, we must select  $t$  such that

$$\max\{t^2\lambda_2^2, t^2r^2 - ntr + \frac{n^2}{4}\} \text{ is smallest possible.}$$

This maximum value is minimized at a root of the quadratic function  $\phi(t) := (t^2r^2 - trn + \frac{n^2}{4}) - t^2\lambda_2^2 = t^2(r^2 - \lambda_2^2) - trn + \frac{n^2}{4}$ . Its discriminant is  $r^2n^2 - n^2(r^2 - \lambda_2^2) = n^2\lambda_2^2$  and  $\phi(t)$  has two roots  $\frac{rn + \varepsilon n\lambda_2}{2(r^2 - \lambda_2^2)} = \frac{n}{2(r - \varepsilon\lambda_2)}$  for  $\varepsilon = \pm 1$ . So  $\max\{t^2\lambda_2^2, t^2r^2 - ntr + \frac{n^2}{4}\}$  is minimized at the smallest root  $t := \frac{n}{2(r + \lambda_2)}$ . Therefore we have  $\widehat{h}(G) = t\lambda_2 = \frac{n\lambda_2}{2(r + \lambda_2)}$ , which proves (7.42).  $\square$

**7.4.2. An eigenvalue-based upper bound  $\widehat{g}(G)$  for  $g(G)$ .** In the same way one can give an eigenvalue-based upper bound  $\widehat{g}(G)$  for the parameter  $g(G)$  when  $G$  is bipartite  $r$ -regular. It is obtained by solving analytically the following optimization problem

$$\widehat{g}(G) := \min_{\lambda, \mu, t \in \mathbb{R}} \left\{ \lambda : \lambda(\mu I - C + tA_G) - \frac{\mu^2}{4}J \succeq 0, \lambda \geq 0 \right\}.$$

**Proposition 7.23.** *Assume  $G$  is a bipartite  $r$ -regular graph, set  $n := |V_1| = |V_2|$ , and let  $\lambda_2$  be the second largest eigenvalue of the adjacency matrix  $A_G$  of  $G$ . Then we have*

$$g_1(G) \leq \widehat{g}(G) = \begin{cases} \frac{n^2\lambda_2^2}{(\lambda_2 + r)^2} & \text{if } r \leq 3\lambda_2, \\ \frac{n^2\lambda_2}{8(r - \lambda_2)} & \text{otherwise.} \end{cases}$$

Moreover, equality  $g_1(G) = \widehat{g}(G)$  holds if  $G$  is vertex- and edge-transitive.

The details of the proof are analogous to those for the parameter  $\widehat{h}(G)$  considered in the previous section, but technically more involved. So we omit the proof. For the reader interested, the proof can be found in my work with Laurent and Polak [LPV23, Appendix C].

**Remark 7.24.** *Here are examples of regular bipartite graphs satisfying  $r \leq 3\lambda_2$ , or the reverse inequality  $3\lambda_2 \leq r$ : If  $G$  is a perfect matching on  $2n$  vertices, then  $\lambda_2 = r = 1$  and thus  $r < 3\lambda_2$  (see Section 7.5.1); on the other hand, if  $G$  is the complete bipartite graph  $K_{n,n}$  minus a perfect matching, then  $r = n - 1$  and  $\lambda_2 = 1$  and thus  $r \geq 3\lambda_2$  if  $n \geq 4$  (see Section 7.5.2).*

Recall the inequalities  $h(G) \leq \frac{1}{2}\sqrt{g(G)}$  (from Lemma 7.1) and  $h_1(G) \leq \frac{1}{2}\sqrt{g_1(G)}$  (from Proposition 7.2). One can check that also the eigenvalue bounds satisfy the analogous relation

$$\widehat{h}(G) \leq \frac{1}{2}\sqrt{\widehat{g}(G)}$$

with equality if and only if  $r \leq 3\lambda_2$ . Hence, in the regime  $3\lambda_2 < r$ , the parameter  $\widehat{h}(G)$  provides a strictly better bound than  $\frac{1}{2}\sqrt{\widehat{g}(G)}$  for both  $h(G)$  and  $\frac{1}{2}\sqrt{g(G)}$ .

So we have

$$h_1(G) \leq \min\{\widehat{h}(G), \frac{1}{2}\sqrt{g_1(G)}\} \leq \max\{\widehat{h}(G), \frac{1}{2}\sqrt{g_1(G)}\} \leq \frac{1}{2}\sqrt{\widehat{g}(G)}.$$

We now observe that the two parameters  $\widehat{h}(G)$  and  $\frac{1}{2}\sqrt{g_1(G)}$  are incomparable. Indeed, as observed above, strict inequality  $\widehat{h}(G) < \frac{1}{2}\sqrt{g_1(G)}$  may hold (e.g., for  $K_{n,n}$  minus a perfect matching). On the other hand, there are regular bipartite graphs satisfying  $\frac{1}{2}\sqrt{g_1(G)} < \widehat{h}(G)$  (such  $G$  is not edge-transitive). As an example, let  $G$  be the disjoint union of  $C_4$  and  $C_6$ , thus 2-regular with  $\lambda_2 = 2$ . Then, we verified that  $\frac{1}{2}\sqrt{g_1(G)} = \frac{1}{2}\sqrt{6} < \frac{5}{4} = \widehat{h}(G)$ .

**7.4.3. Links to some other eigenvalue bounds.** In this section, we investigate links between the new bounds introduced in previous sections and some known eigenvalue bounds in the literature. First, we point out a natural link between  $\widehat{h}(\cdot)$  and Hoffman’s ratio bound (7.44) for the stability number of a graph. After that, we present links to some spectral parameters  $\varphi(G)$ ,  $\varphi'(G)$  and  $\varphi_H(G)$  by Haemers [Haem97, Haem01], which he used to bound the parameter  $g_{bc}(G)$ , the maximum number of edges in a biclique of an arbitrary graph  $G$ ; see (7.46), (7.49) and (7.52) below for the exact definitions. As the equality  $g_{bc}(G) = g_{bi}(\overline{G}) = g(B_0(\overline{G}))$  holds, also the parameter  $h_1(B_0(\overline{G}))$  provides an upper bound for  $g_{bc}(G)$ . We will review the parameters of Haemers and investigate their relationships with the parameters  $h_1(\cdot)$  and  $\widehat{h}(\cdot)$ .

**Linking the parameter  $\widehat{h}(B(G))$  to Hoffman’s bound for  $\alpha(G)$ .** Let  $G = (V = [n], E)$  be an arbitrary graph and let  $\lambda_n(A_G)$  be the smallest eigenvalue of its adjacency matrix. If  $G$  is  $r$ -regular, then the following bound holds for its stability number:

$$\alpha(G) \leq n \frac{-\lambda_n(A_G)}{r - \lambda_n(A_G)}. \tag{7.44}$$

This bound was proved by Hoffman (unpublished) and is known as Hoffman’s ratio bound (see Haemers [Haem21] for a short proof and a historical account). There is a tight link between Hoffman’s ratio bound for  $G$  and the parameter  $\widehat{h}(\cdot)$  for its bipartite double  $B(G)$ . Indeed, if  $A \subseteq V$  is an independent set in  $G$ , then the pair  $(A, A)$  is a balanced biindependent pair in  $B(G)$ . So  $|A| \leq \alpha(G)$  and  $2|A| \leq \alpha_{bal}(B(G)) \leq 4 \cdot \widehat{h}(B(G))$ , giving

$$\alpha(G) \leq \frac{1}{2}\alpha_{bal}(B(G)) \leq 2 \cdot \widehat{h}(B(G)) = n \frac{\lambda_2(A_{B(G)})}{r + \lambda_2(A_{B(G)})}. \tag{7.45}$$

By Lemma 7.21, we have  $\lambda_2(A_{B(G)}) = \max\{\lambda_2(A_G), -\lambda_n(A_G)\}$ , and thus

$$n \frac{-\lambda_n(A_G)}{r - \lambda_n(A_G)} \leq 2 \cdot \widehat{h}(B(G)) = n \frac{\lambda_2(A_{B(G)})}{r + \lambda_2(A_{B(G)})}.$$

Lovász [Lov79] showed that also  $\vartheta(G)$  is upper bounded by Hoffman’s ratio bound. The parameters  $\vartheta(G)$  and  $h_1(B(G))$  satisfy the analogous relationship:

$$\vartheta(G) \leq 2 \cdot h_1(B(G)).$$

Indeed, if  $X$  is an optimal solution to program (3.1), then  $X' := \frac{1}{2} \begin{pmatrix} X & X \\ X & X \end{pmatrix}$  is feasible for (7.28) with objective value  $\langle C, X' \rangle = \frac{1}{2} \langle J, X \rangle = \frac{1}{2} \vartheta(G)$ , giving the desired inequality.

**Linking the parameter  $h_1(B_0(G))$  to Haemers’ bound  $\varphi(G)$ .** As we saw earlier, for any bipartite graph  $G$ , the parameter  $h_1(G)$  provides an upper bound for the parameter  $g(G)$ , via  $\frac{1}{2} \sqrt{g(G)} \leq h_1(G)$ . This also directly gives a bound for the parameter  $g_{bi}(G) = g(B_0(G))$  when  $G$  is an arbitrary graph, namely  $\frac{1}{2} \sqrt{g_{bi}(G)} \leq h_1(B_0(G))$ .

For an arbitrary graph  $G = (V, E)$ , Haemers [Haem01] introduced the spectral parameter

$$\varphi(G) := \min_{M \in \mathcal{S}^{|V|}} \{ \lambda_{abs}(M) : M_{ij} = 1 \text{ for all } \{i, j\} \in E \}, \tag{7.46}$$

where  $\lambda_{abs}(M)$  denotes the maximum absolute value of an eigenvalue of  $M$ , and he shows that  $\varphi(G)$  provides an upper bound for the parameter  $g_{bc}(G) = g_{bi}(\overline{G})$  via the inequality

$$\sqrt{g_{bc}(G)} \leq \varphi(G). \tag{7.47}$$

So we have two bounds for  $g_{bc}(G)$ , namely  $\frac{1}{2} \sqrt{g_{bc}(G)} \leq \frac{1}{2} \varphi(G)$  and  $\frac{1}{2} \sqrt{g_{bc}(G)} \leq h_1(B_0(\overline{G}))$ . We now show that these two upper bounds in fact coincide.

**Lemma 7.25.** *For any graph  $G$ , we have  $h_1(B_0(G)) = \frac{1}{2} \varphi(\overline{G})$ .*

PROOF. Let  $G = (V, E)$  and  $\overline{G} = (V, \overline{E})$ . First observe the parameter  $\varphi(\overline{G})$  can be reformulated as

$$\varphi(\overline{G}) = \min \left\{ \lambda_{\max}(Y) : Y = \begin{pmatrix} 0 & M \\ M & 0 \end{pmatrix}, M \in \mathcal{S}^{|V|}, M_{ij} = 1 \text{ for } \{i, j\} \in \overline{E} \right\}; \tag{7.48}$$

this follows from the fact that the eigenvalues of any  $Y$  in (7.48) are  $\pm \lambda_i(M)$  for  $i \in [|V|]$ . Let  $V \cup V'$  be the vertex set of the extended bipartite double  $B_0(G)$ , where  $V'$  is a disjoint copy of  $V$ , and let  $C$  be the matrix from (7.21), which is now indexed by  $V \cup V'$ . We use the formulation (7.27) of  $h_1(B_0(G))$ , defined as the smallest scalar  $\lambda$  for which  $\lambda I - C + Z \succeq 0$  for some  $Z \in \mathcal{S}_{B_0(G)}$  or, equivalently, as the minimum value of  $\lambda_{\max}(C - Z)$  for  $Z \in \mathcal{S}_{B_0(G)}$ . Since the condition  $Z \in \mathcal{S}_{B_0(G)}$  corresponds to  $Y := 2(C - Z)$  being feasible for (7.48), we can conclude that  $2h_1(B_0(G)) = \varphi(\overline{G})$ . □

**Linking  $h_1(B_0(G))$  to Haemers' spectral bounds  $\varphi'(G)$  and  $\varphi_H(G)$ .** In the previous section we mentioned the spectral bound  $\varphi(G)$  from (7.46) of Haemers [Haem01] for the parameter  $g_{bc}(G)$  and observed its link to the parameter  $h_1(\cdot)$ , recall (7.47) and Lemma 7.25. In some earlier work [Haem97], Haemers introduced the following spectral parameter for an arbitrary graph  $G = (V = [n], E)$ ,

$$\varphi'(G) := \min_{M \in \mathcal{S}^{|V|}} \left\{ n \frac{\lambda(M)}{1 + \lambda(M)} : Me = e, M_{ij} = 0 \text{ for } \{i, j\} \in E \right\}, \quad (7.49)$$

where  $\lambda(M)$  denotes the second largest absolute value of an eigenvalue of  $M$ . Haemers [Haem01] showed that  $\varphi(G) \leq \varphi'(G)$  for all  $G$  and that there are graphs  $G$  for which the inequality is strict.

Let  $L_G$  denote the Laplacian matrix of  $G$  that is defined as  $L_G = D_G - A_G$ , where  $D_G \in \mathcal{S}^n$  is the diagonal matrix whose  $i$ -th entry is the degree of vertex  $i \in V$  in  $G$ . In what follows we let  $0 = \mu_1 \leq \mu_2 \leq \dots \leq \mu_n$  denote the eigenvalues of the Laplacian matrix  $L_G$ . In [Haem97, Theorem 2.4] Haemers shows the inequality

$$\varphi'(\overline{G}) \leq \varphi_H(G) := \frac{n}{2} \left( 1 - \frac{\mu_2}{\mu_n} \right) \quad (7.50)$$

for any graph  $G$  (on  $n$  nodes), and he shows that equality holds in (7.50) if  $G$  is vertex- and edge-transitive. So we have the following inequalities

$$(h_1(B_0(G))) = \frac{1}{2} \varphi(\overline{G}) \leq \frac{1}{2} \varphi'(\overline{G}) \leq \frac{1}{2} \varphi_H(G) = \frac{n}{4} \left( 1 - \frac{\mu_2}{\mu_n} \right), \quad (7.51)$$

where the right most inequality is an equality if  $G$  is vertex- and edge-transitive. We next sharpen this latter result and show that  $h_1(B_0(G)) = \frac{n}{4} \left( 1 - \frac{\mu_2}{\mu_n} \right)$  if  $G$  is vertex- and edge-transitive.

**Proposition 7.26.** *Let  $G = (V, E)$  be a graph, set  $n := |V|$ , and let  $0 = \mu_1 \leq \mu_2 \leq \dots \leq \mu_n$  denote the eigenvalues of the Laplacian matrix of  $G$ . Then we have*

$$h_1(B_0(G)) = \frac{1}{2} \varphi(\overline{G}) \leq \frac{1}{2} \varphi_H(G) = \frac{n}{4} \left( 1 - \frac{\mu_2}{\mu_n} \right),$$

*with equality if  $G$  is vertex- and edge-transitive.*

**PROOF.** Consider the parameter  $\tilde{h}(G)$  obtained from the definition of  $h_1(B_0(G))$  in (7.27), where we restrict the optimization to matrices  $Z$  of the form  $Z = \begin{pmatrix} 0 & tL_G + \mu I \\ tL_G + \mu I & 0 \end{pmatrix}$  for scalars  $t, \mu \in \mathbb{R}$ . Hence,  $h_1(B_0(G)) \leq \tilde{h}(G)$ . First, we show that if  $G$  is vertex- and edge-transitive (hence regular), then this restriction can be made without loss of generality and thus  $h_1(B_0(G)) = \tilde{h}(G)$ .

For this, for any permutation  $\sigma$  of  $V$  consider the associated permutation  $\tilde{\sigma}$  of  $V \cup V'$  (the vertex set of  $B_0(G)$ , where  $V'$  is a disjoint copy of  $V$ ) defined by  $\tilde{\sigma}(i) = \sigma(i)$  and  $\tilde{\sigma}(i') := \sigma(i)'$  for  $i \in V$ ; clearly,  $\tilde{\sigma}$  is an automorphism of  $B_0(G)$  if  $\sigma$  is an automorphism of  $G$ . Consider in addition the automorphism  $\pi$  of

$B_0(G)$  obtained by flipping  $V$  and  $V'$ :  $\pi(i) = i'$  and  $\pi(i') = i$  for  $i \in V$ . Then, under the action of the group of automorphisms of  $B_0(G)$  generated by  $\pi$  and  $\tilde{\sigma}$  (for  $\sigma$  automorphism of  $G$ ), the edge set of  $B_0(G)$  is partitioned into two orbits, the orbit  $\Omega_V := \{\{i, i'\} : i \in V\}$  and the orbit  $\Omega_E := \{\{i, j'\}, \{i', j\} : \{i, j\} \in E\}$ . Now, if  $(\lambda, Z)$  is feasible for  $h_1(B_0(G))$ , then the same holds for its symmetrization obtained by averaging over the group of automorphisms of  $B_0(G)$  just described. This gives a new feasible solution  $(\lambda, Z)$ , where the entries of  $Z$  take two possible nonzero values, depending whether the entry corresponds to an edge in  $\Omega_V$  or in  $\Omega_E$ , and thus  $Z$  has indeed the desired form claimed above.

We now aim to compute the optimum value of the program

$$\tilde{h}(G) = \min_{\lambda, t, \mu \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda I & tL_G + \mu I - \frac{1}{2}J \\ tL_G + \mu I - \frac{1}{2}J & \lambda I \end{pmatrix} \succeq 0 \right\}$$

and to show it is equal to  $\frac{n}{4} \left(1 - \frac{\mu_2}{\mu_n}\right)$ . By taking a Schur complement (and assuming  $\lambda > 0$ ) the matrix in the above semidefinite program is positive semidefinite if and only if the matrix

$$\begin{aligned} & \lambda^2 I - (tL_G + \mu I - \frac{1}{2}J)(tL_G + \mu I - \frac{1}{2}J) \\ & = (\lambda^2 - \mu^2)I - t^2 L_G^2 - 2t\mu L_G + (\mu - \frac{n}{4})J =: Q \end{aligned}$$

is positive semidefinite. Let  $e$  denote the all-ones vector, which is an eigenvector of  $L_G$  for its smallest eigenvalue  $\mu_1 = 0$ , and let  $w_i \perp e$  be an eigenvector of  $L_G$  for its eigenvalue  $\mu_i$  with  $i \geq 2$ . Then the eigenvalues of  $Q$  at these eigenvectors are as follows:

$$\begin{aligned} \text{at } e: & \quad \lambda^2 - \mu^2 + n(\mu - \frac{n}{4}) = \lambda^2 - (\mu - \frac{n}{2})^2, \\ \text{at } w_i \perp e: & \quad \lambda^2 - (t\mu_i + \mu)^2, \quad \text{for } i = 2, \dots, n. \end{aligned}$$

Hence  $Q \succeq 0$  if and only if all these eigenvalues are nonnegative and thus we must select  $t, \mu$  such that

$$\max \left\{ (\mu - \frac{n}{2})^2, (t\mu_2 + \mu)^2, (t\mu_n + \mu)^2 \right\} \text{ is smallest possible.}$$

So we must find the smallest value of  $\lambda$  for which there exist  $t, \mu$  satisfying the system

$$\lambda \geq |t\mu_2 + \mu|, \quad \lambda \geq |t\mu_n + \mu|, \quad \lambda \geq |\mu - \frac{n}{2}|.$$

First, note that taking  $\mu := \frac{n}{4} + \frac{n\mu_2}{4\mu_n}$ ,  $t := \frac{-n}{2\mu_n}$  and  $\lambda := \frac{n}{4} \left(1 - \frac{\mu_2}{\mu_n}\right)$  is feasible for the above system (since  $t\mu_2 + \mu = \lambda$ ,  $t\mu_n + \mu = \mu - \frac{n}{2} = -\lambda$ ), which shows  $\tilde{h}(G) \leq \frac{n}{4} \left(1 - \frac{\mu_2}{\mu_n}\right)$ . We now show the reverse inequality. Assume  $\lambda, t, \mu$  satisfy the above system. The conditions  $\lambda \geq -t\mu_n - \mu$  and  $\lambda \geq t\mu_2 + \mu$  together give  $\lambda \geq \frac{1}{2}(\mu_2 - \mu_n)t$ , and the conditions  $\lambda \geq t\mu_2 + \mu$  and  $\lambda \geq -\mu + \frac{n}{2}$  give  $\lambda \geq \frac{\mu_2}{2}t + \frac{n}{4}$ . Therefore,  $\tilde{h}(G)$  is at least the smallest value of  $\lambda$  for which there exists  $t$  such that  $\lambda \geq \max\{\frac{1}{2}(\mu_2 - \mu_n)t, \frac{\mu_2}{2}t + \frac{n}{4}\}$ . Now observe that this maximum

is minimized at the intersection point, where  $t = -\frac{n}{2\mu_n}$  (since  $\mu_2 - \mu_n \leq 0$  and  $\mu_2 \geq 0$ ). This gives the desired relation  $\tilde{h}(G) \geq \frac{1}{2}(\mu_2 - \mu_n)\left(\frac{n}{-2\mu_n}\right) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$ , which concludes the proof.  $\square$

An interesting feature of the closed-form bound  $\frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right)$  in Proposition 7.26 is that it is valid without any regularity assumption on the graph  $G$ .

Assume now  $G$  is  $r$ -regular, still arbitrary (not necessarily bipartite) on  $n$  nodes. Then its adjacency matrix  $A_G$  satisfies  $A_G = rI - L_G$  and thus its eigenvalues are  $\lambda_i = r - \mu_i$  for  $i \in [n]$ , with  $\lambda_1 = r \geq \lambda_2 \geq \dots \geq \lambda_n$ . Therefore, for any  $r$ -regular graph  $G$ , we have

$$h_1(B_0(G)) \leq \frac{1}{2}\varphi_H(G) = \frac{n}{4}\left(1 - \frac{\mu_2}{\mu_n}\right) = \frac{n}{4}\frac{\lambda_2 - \lambda_n}{r - \lambda_n}. \quad (7.52)$$

As shown in Proposition 7.26, equality  $h_1(B_0(G)) = \frac{1}{2}\varphi_H(G)$  holds if  $G$  is vertex- and edge-transitive. Since the extended bipartite double graph  $B_0(G)$  is  $(r+1)$ -regular, one can also upper bound  $h_1(B_0(G))$  by the parameter  $\hat{h}(B_0(G))$  (as defined in Proposition 7.3). By Lemma 7.21, the second largest eigenvalue of the adjacency matrix of  $B_0(G)$  equals  $\max\{\lambda_2 + 1, -\lambda_n - 1\}$ , and thus

$$h_1(B_0(G)) \leq \hat{h}(B_0(G)) = \frac{n}{2}\frac{\max\{\lambda_2 + 1, -\lambda_n - 1\}}{\max\{\lambda_2 + 1, -\lambda_n - 1\} + r + 1}. \quad (7.53)$$

Next we compare the upper bounds in (7.52) and (7.53).

**Proposition 7.27.** *Let  $G$  be an  $r$ -regular graph. Then,  $\frac{1}{2}\varphi_H(G) \leq \hat{h}(B_0(G))$ , with equality if and only if  $\lambda_2 = r$  or  $\lambda_2 + \lambda_n + 2 = 0$ .*

PROOF. Set  $\mu := \max\{\lambda_2 + 1, -\lambda_n - 1\}$  and note that  $\frac{1}{2}\varphi_H(G) \leq \hat{h}(B_0(G))$  is equivalent to  $\psi := \mu(\lambda_2 + \lambda_n - 2r) + (r+1)(\lambda_2 - \lambda_n) \leq 0$ . If  $\lambda_2 + \lambda_n + 2 \geq 0$  then  $\mu = \lambda_2 + 1$  and we have  $\psi = (\lambda_2 - r)(\lambda_2 + \lambda_n + 2) \leq 0$ . Otherwise,  $\lambda_2 + \lambda_n + 2 \leq 0$ ,  $\mu = -\lambda_n - 1$  and we have  $\psi = (r - \lambda_2)(\lambda_2 + \lambda_n + 2) \leq 0$ .  $\square$

So, Haemers' bound  $\varphi_H(G)$  improves on the bound  $\hat{h}(B_0(G))$  for any regular graph  $G$ . On the other hand, also the reverse situation may occur, where the parameter  $\hat{h}$  improves on Haemers' bound  $\varphi_H$ . For this consider a bipartite graph  $G = (V_1 \cup V_2, E)$ . As observed in (7.7), we have  $g_{bc}(G) = g(\overline{G}^b)$ , where  $\overline{G}^b = (V_1 \cup V_2, (V_1 \times V_2) \setminus E)$  is the bipartite complement of  $G$ . Hence we have the inequalities

$$\begin{aligned} \frac{1}{2}\sqrt{g_{bc}(G)} &= \frac{1}{2}\sqrt{g(\overline{G}^b)} \leq h_1(\overline{G}^b) \leq \hat{h}(\overline{G}^b), \\ \frac{1}{2}\sqrt{g_{bc}(G)} &= \frac{1}{2}\sqrt{g(B_0(\overline{G}))} \leq h_1(B_0(\overline{G})) \leq \frac{1}{2}\varphi_H(\overline{G}), \end{aligned} \quad (7.54)$$

where we assume that  $G$  is regular when considering the parameters  $\widehat{h}(\overline{G}^b)$  and  $\varphi_H(\overline{G})$ . Next we show that  $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$  and that  $\widehat{h}(\overline{G}^b) \leq \frac{1}{2}\varphi_H(\overline{G})$ .

**Proposition 7.28.** *Let  $G$  be a bipartite graph. Then we have  $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$ . Moreover, if  $G$  is  $r$ -regular,  $n := |V_1| = |V_2|$  and  $\lambda_2$  denotes the second largest eigenvalue of  $A_G$ , then we have*

$$\widehat{h}(\overline{G}^b) = \frac{n}{2} \frac{\lambda_2}{\lambda_2 + n - r} \leq \frac{1}{2} \varphi_H(\overline{G}) = \frac{n}{2} \frac{\lambda_2 + r}{2n - r + \lambda_2}, \tag{7.55}$$

with strict inequality precisely when  $\lambda_2 < r < n$ , i.e., when  $G$  is connected and  $G \neq K_{n,n}$ .

PROOF. First, we prove  $h_1(B_0(\overline{G})) = h_1(\overline{G}^b)$ . For this, we use the formulation (7.28) for the parameter  $h_1(\cdot)$ . Recall the definition (7.21) of the matrix  $C \in \mathcal{S}^{|V|}$  for the bipartition  $V = V_1 \cup V_2$ , and let  $\widetilde{C} \in \mathcal{S}^{|V|+|V'|}$  denote the analogous matrix corresponding now to the bipartition  $V \cup V'$ , where  $V = V_1 \cup V_2$  and  $V' = V'_1 \cup V'_2$  is a disjoint copy of  $V$ . The matrices  $\widetilde{C}$  and  $A_{B_0(\overline{G})}$  have the form

$$\widetilde{C} = \frac{1}{2} \begin{pmatrix} 0 & J & J & 0 \\ J & 0 & 0 & J \\ J & 0 & 0 & J \\ 0 & J & J & 0 \end{pmatrix} \text{ and } A_{B_0(\overline{G})} = \begin{pmatrix} 0 & A(\overline{G}^b) & I & 0 \\ A(\overline{G}^b) & 0 & 0 & I \\ I & 0 & 0 & A(\overline{G}^b) \\ 0 & I & A(\overline{G}^b) & 0 \end{pmatrix} \text{ with respect}$$

to the partition  $V_1 \cup V'_2 \cup V'_1 \cup V_2$  (taken in that order), setting  $A(\overline{G}^b) := A_{\overline{G}^b}$  for easier notation. If  $X \in \mathcal{S}^{|V|}$  is optimal for  $h_1(\overline{G}^b)$ , then  $Y := \frac{1}{2} \begin{pmatrix} X & 0 \\ 0 & X \end{pmatrix}$  is feasible for  $h_1(B_0(\overline{G}))$  with  $\langle \widetilde{C}, Y \rangle = \langle C, X \rangle$ , which shows  $h_1(B_0(\overline{G})) \geq h_1(\overline{G}^b)$ . Conversely, assume  $Y \in \mathcal{S}^{|V|+|V'|}$  is optimal for  $h_1(B_0(\overline{G}))$ . Let  $X$  (resp.,  $X'$ ) denote the principal submatrix of  $Y$  indexed by  $V_1 \cup V'_2$  (resp.,  $V'_1 \cup V_2$ ). Then  $X/\text{Tr}(X)$  and  $X'/\text{Tr}(X')$  are both feasible for  $h_1(\overline{G}^b)$ , which implies  $h_1(\overline{G}^b) \cdot \text{Tr}(X) \geq \langle C, X \rangle$  and  $h_1(\overline{G}^b) \cdot \text{Tr}(X') \geq \langle C, X' \rangle$ . Summing up and using  $\text{Tr}(X) + \text{Tr}(X') = \text{Tr}(Y) = 1$ , we get  $h_1(\overline{G}^b) \geq \langle C, X \rangle + \langle C, X' \rangle = \langle \widetilde{C}, Y \rangle = h_1(B_0(\overline{G}))$ .

Assume now  $G$  is bipartite  $r$ -regular,  $\lambda_2 = \lambda_2(A_G)$  and  $n := |V_1| = |V_2|$ ; we show (7.55). First we compute the parameter  $\widehat{h}(\overline{G}^b)$ . For this note that  $\overline{G}^b$  is  $(n - r)$ -regular. Moreover, if  $M_G$  denotes the incidence matrix of  $G$ , then the incidence matrix of  $\overline{G}^b$  is  $J - M_G$ , whose second largest singular value is equal to the second largest singular value of  $M_G$  and thus to  $\lambda_2$ . Hence, using relation (7.42), we obtain  $\widehat{h}(\overline{G}^b) = \frac{n}{2} \frac{\lambda_2}{n - r + \lambda_2}$ , as desired. Next we compute the parameter  $\varphi_H(\overline{G})$ . For this note that  $\overline{G}$  is  $(2n - 1 - r)$ -regular, the second largest eigenvalue of  $A_{\overline{G}}$  is  $-1 - \lambda_{\min}(A_G) = r - 1$  and its smallest eigenvalue is  $-1 - \lambda_2(A_G) = -1 - \lambda_2$ . In view of (7.52) we get  $\varphi_H(\overline{G}) = n \frac{r + \lambda_2}{2n - r + \lambda_2}$ , as desired. One can then easily check that the inequality in (7.55) is equivalent to  $(r - \lambda_2)(n - r) \geq 0$ , which holds since  $\lambda_2 \leq r \leq n$ . Hence the inequality

$$\begin{array}{c}
 \text{with equality if } \overline{G} \text{ is vertex-} \\
 \text{and edge-transitive} \\
 \text{Prop. 7.26} \\
 \frac{1}{2} \sqrt{g_{bc}(G)} \leq \overbrace{h_1(B_0(\overline{G}))} \leq \frac{1}{2} \varphi_H(\overline{G}) \leq \widehat{h}(B_0(\overline{G})) \\
 \text{with equality if and only if} \\
 \lambda_n = r - n \text{ or } \lambda_2 + \lambda_n = 0 \\
 \text{Prop. 7.27}
 \end{array}$$

FIGURE 7.2. Bounds on  $g_{bc}(G)$  for  $G$   $r$ -regular

$$\begin{array}{c}
 \text{with equality if and only if} \\
 \lambda_2 = r \text{ or } r = n \\
 \text{Prop 7.28} \\
 \frac{1}{2} \sqrt{g_{bc}(G)} \leq \underbrace{h_1(B_0(\overline{G})) = h_1(\overline{G}^b)}_{\text{Prop. 7.28}} \leq \widehat{h}(\overline{G}^b) \leq \frac{1}{2} \varphi_H(\overline{G}) \leq \widehat{h}(B_0(\overline{G})) \\
 \text{with equality if and only if} \\
 \lambda_n = r - n \text{ or } \lambda_2 + \lambda_n = 0 \\
 \text{Prop. 7.27}
 \end{array}$$

FIGURE 7.3. Bounds on  $g_{bc}(G)$  for  $G$  bipartite  $r$ -regular

in (7.55) is strict precisely when  $\lambda_2 < r < n$ , i.e., when  $G$  is connected and  $G \neq K_{n,n}$ . □

We summarize the various bounds obtained above for the parameter  $g_{bc}(G)$  when  $G$  is an arbitrary  $r$ -regular graph (Figure 7.2) and when  $G$  is bipartite  $r$ -regular (Figure 7.3). As before, let  $\lambda_1 = r \geq \lambda_2 \geq \dots \geq \lambda_n$  denote the eigenvalues of  $A_G$ . Then,  $\overline{G}$  is  $(n - 1 - r)$ -regular, with  $\lambda_2(A_{\overline{G}}) = -1 - \lambda_n$  and  $\lambda_n(A_{\overline{G}}) = -1 - \lambda_2$ .

### 7.5. Examples

We now illustrate the behaviour of the various parameters discussed above on some classes of regular graphs. Recall the definition of the matrix  $M_G$  in Lemma 7.21.

**7.5.1. The perfect matching.** For  $n \geq 2$ , let  $G$  be a perfect matching on  $2n$  vertices. Then,  $M_G = I$ ,  $r = 1$ ,  $\lambda_2 = 1$ , and  $G$  is vertex- and edge-transitive. Using Proposition 7.3 we obtain

$$h_1(G) = \widehat{h}(G) = \frac{n}{2} \frac{\lambda_2}{r + \lambda_2} = \frac{n}{4} \quad \text{and} \quad g_1(G) = \widehat{g}(G) = \frac{n^2}{4}.$$

We have  $g(G) = \lfloor n/2 \rfloor \lceil n/2 \rceil$  and  $h(G) = \frac{1}{n} \lfloor n/2 \rfloor \lceil n/2 \rceil$  (obtained by maximizing  $ab$  and  $\frac{ab}{a+b}$  with  $a, b \geq 0$  integers and  $a+b \leq n$ ). Hence,  $h_1(G) = \frac{1}{2} \sqrt{g_1(G)}$  and  $h_1(G), g_1(G)$  give tight bounds for  $h(G), g(G)$  (with equality for  $n$  even and up to rounding for  $n$  odd).



**7.5.2. The complete bipartite graph  $K_{n,n}$  minus a perfect matching.** For  $n \geq 2$ , let  $G$  be the complete bipartite graph  $K_{n,n}$  with a deleted perfect matching (also known as the *crown graph* on  $2n$  vertices). Then  $G$  is vertex- and edge-transitive,  $(n - 1)$ -regular,  $M_G = J_n - I_n$ , and  $\lambda_2 = 1$ . We have  $h(G) = \frac{1}{2}$  and  $g(G) = 1$ . Using Proposition 7.3 we obtain

$$h_1(G) = \widehat{h}(G) = \frac{n}{2} \frac{\lambda_2}{r + \lambda_2} = \frac{1}{2}, \quad \text{and} \quad g_1(G) = \widehat{g}(G) = \begin{cases} \frac{n^2}{8(n-2)} & n \geq 4, \\ 1 & n \leq 4. \end{cases}$$

Hence the bound  $h_1(G)$  is tight for both  $h(G)$  and  $\frac{1}{2}\sqrt{g(G)}$ , while the ratio  $g_1(G)/g(G)$  grows linearly in  $n$ . Note that  $h_1(G) < \frac{1}{2}\sqrt{g_1(G)}$  for  $n \geq 5$ , which gives an example with strict separation between the parameters  $h_1$  and  $\frac{1}{2}\sqrt{g_1}$  (and thus  $\widehat{h}$  and  $\frac{1}{2}\sqrt{\widehat{g}}$ ). In view of (7.54), the parameter  $g_{bc}(G)$  is upper bounded by  $4\widehat{h}(\overline{G}^b)^2$  and by  $\varphi_H(\overline{G})^2$ . Note that  $4\widehat{h}(\overline{G}^b)^2 = 4(\frac{n}{4})^2 = \frac{n^2}{4}$ , which improves on Haemers' bound  $\varphi_H(\overline{G})^2 = (\frac{n^2}{n+2})^2$  for  $n \geq 3$ . This thus gives a class of graphs for which strict inequality holds in (7.55).

**7.5.3. The cycle graph  $C_n$ .** Let  $G$  be the cycle  $C_n$  on  $n \geq 3$  vertices, which is vertex- and edge-transitive, and 2-regular. The eigenvalues of the adjacency matrix  $A_{C_n}$  are  $2\cos(2\pi j/n)$  where  $j = 0, \dots, n - 1$  (see, e.g., [BH17]), so  $\lambda_2(A_{C_n}) = 2\cos(2\pi/n)$ , and  $\lambda_n(A_{C_n}) = -2$  if  $n$  is even,  $\lambda_n(A_{C_n}) = -2\cos(\pi/n)$  if  $n$  is odd.

First, we compute the parameters for the extended bipartite double graph  $B_0(C_n)$ . Using Proposition 7.26 and relations (7.52), (7.53), we get

$$h_1(B_0(C_n)) = \frac{1}{2}\varphi_H(C_n) = \begin{cases} \frac{n}{4}\cos(\pi/n)^2 & \text{if } n \text{ even,} \\ \frac{n}{4}(2\cos(\pi/n) - 1) & \text{if } n \text{ odd,} \end{cases} \quad (7.56)$$

$$\widehat{h}(B_0(C_n)) = \frac{n}{4} \frac{2\cos(2\pi/n) + 1}{\cos(2\pi/n) + 2}. \quad (7.57)$$

Hence, we have  $h_1(B_0(C_n)) = \widehat{h}(B_0(C_n)) (= 0)$  for  $n = 3$  (in which case  $B_0(C_3) = K_{3,3}$ ), and strict inequality  $h_1(B_0(C_n)) < \widehat{h}(B_0(C_n))$  for  $n \geq 4$  (as expected from Proposition 7.27). Note also that  $B_0(C_n)$  is not edge-transitive if  $n \geq 4$ . One can also show that

$$h(B_0(C_n)) = \begin{cases} \frac{1}{4}(n - 2) & \text{if } n \text{ even,} \\ \frac{(n-1)(n-3)}{4(n-2)} & \text{if } n \text{ odd,} \end{cases}$$

$$g(B_0(C_n)) = \begin{cases} \frac{1}{4}(n - 2)^2 & \text{if } n \text{ even,} \\ \frac{1}{4}(n - 1)(n - 3) & \text{if } n \text{ odd.} \end{cases}$$

So  $h(B_0(C_n)) \leq \frac{1}{2}\sqrt{g(B_0(C_n))}$ , with equality for  $n$  even. Moreover, the ratio  $\widehat{h}(B_0(C_n))/h(B_0(C_n))$  tends to 1 as  $n \rightarrow \infty$ , so the bound  $\widehat{h}(B_0(C_n))$  (and thus  $h_1(B_0(C_n))$  too) is asymptotically tight for  $h(B_0(C_n))$  and  $\frac{1}{2}\sqrt{g(B_0(C_n))}$ .

For  $n$  even the graph  $G = C_n$  is bipartite. Then we have

$$h(C_n) \leq h_1(C_n) = \widehat{h}(C_n) = \frac{n}{4} \frac{\lambda_2}{\lambda_2 + r} = \frac{n}{4} \frac{\cos(2\pi/n)}{\cos(2\pi/n) + 1} \leq \frac{\alpha(C_n)}{4} = \frac{n}{8}.$$

So  $h_1(C_n) = \Theta(n/8) = \Theta(\alpha(C_n)/4)$ . Moreover, one can construct a bipartite biindependent pair  $(A, B)$  showing  $h(C_n) = \Theta(n/8)$  (see also [CLZXL21]). Namely, for  $n \equiv 0 \pmod{4}$ , set  $A = \{1, 3, \dots, \frac{n}{2} - 1\}$ ,  $B = \{\frac{n}{2} + 2, \frac{n}{2} + 4, \dots, n - 2\}$  with  $|A| = \frac{n}{4}$ ,  $|B| = \frac{n}{4} - 1$ , and, for  $n \equiv 2 \pmod{4}$ , set  $A = \{1, 3, \dots, \frac{n}{2} - 2\}$ ,  $B = \{\frac{n}{2} + 1, \frac{n}{2} + 3, \dots, n - 2\}$  with  $|A| = |B| = \frac{n-2}{4}$ .

**7.5.4. The hypercube graph  $Q_r$ .** The hypercube graph  $Q_r$  is the bipartite graph with vertex set  $V = \{0, 1\}^r$ , where two vertices are adjacent when their Hamming distance is 1. So the bipartition is  $V = V_1 \cup V_2$ , where  $V_1$  (resp.,  $V_2$ ) consists of all  $x \in V$  with an even (resp., odd) Hamming weight  $|x|$ . The graph  $Q_r$  is vertex- and edge-transitive, and  $r$ -regular. The eigenvalues of  $A_{Q_r}$  are  $r - 2k$  for  $k = 0, \dots, r$ , where the eigenvalue  $r - 2k$  has multiplicity  $\binom{r}{k}$ . So  $\lambda_2(A_{Q_r}) = r - 2$ . Thus the parameter  $h_1(Q_r)$  is given by

$$h_1(Q_r) = \widehat{h}(Q_r) = 2^{r-3} \frac{r-2}{r-1}.$$

One can show that  $\lim_{r \rightarrow \infty} h_1(Q_r)/h(Q_r) = 1$ . For this, we will show that  $h(Q_r) \geq \frac{a(r-1)}{4}$ , where the sequence  $(a(r))_{r \geq 0}$  is defined recursively by

$$a(2r) := 2^{2r} - \binom{2r}{r}, \quad a(2r+1) := 2 \cdot a(2r) \text{ if } r \geq 1, \text{ and } a(0) = 0. \quad (7.58)$$

Using the fact that  $\binom{2r}{r} \sim \frac{2^{2r}}{\sqrt{\pi r}}$  one can check that  $a(r-1) \sim 2^{r-1}$  and  $h(Q_r) \geq 2^{r-3}(1 - c/\sqrt{r})$  (for some constant  $c > 0$ ) and thus  $h_1(Q_r)/h(Q_r)$  tends to 1 as  $r \rightarrow \infty$ . Note that the bound  $h(Q_r) \leq \alpha(Q_r)/4 = 2^{r-1}/4 = 2^{r-3}$  from Lemma 7.1 is slightly weaker than  $h(Q_r) \leq h_1(Q_r)$ , but already strong enough to exhibit  $h(Q_r) \sim 2^{r-3}$  (when combined with the lower bound  $h(Q_r) \geq \frac{a(r-1)}{4}$ ).

We now show that

$$h(Q_r) \geq \frac{a(r-1)}{4}.$$

For this, it is useful to observe that the graph  $Q_r$  is isomorphic to  $B_0(Q_{r-1})$ , the extended bipartite double of  $Q_{r-1}$  (the bipartition of  $Q_r$  provides the bipartition of  $B_0(Q_{r-1})$  by simply deleting the last coordinate in all vertices of  $Q_r$ ). Thus we have

$$h(Q_r) = h(B_0(Q_{r-1})) = h_{\text{bi}}(Q_{r-1}),$$

where the last equality follows from (7.5). Hence, instead of searching for bipartite biindependent pairs in  $Q_r$ , we may as well search for (general) biindependent pairs in  $Q_{r-1}$ , which is a simpler task. We show that  $h_{\text{bi}}(Q_r) \geq \frac{1}{4}a(r)$

for all  $r \geq 1$ . First consider the case of  $Q_{2r}$ . Define the sets

$$L := \{x \in \{0, 1\}^{2r} : |x| \leq r - 1\}, \quad U := \{x \in \{0, 1\}^{2r} : |x| \geq r + 1\}.$$

Then,  $(L, U)$  is a (balanced) biindependent pair in  $Q_{2r}$ , with  $|L| = |U| = \frac{1}{2}(2^{2r} - \binom{2r}{r}) = \frac{1}{2}a(2r)$ , which implies  $h_{\text{bi}}(Q_r) \geq \frac{1}{4}a(2r)$ . Consider now the case of  $Q_{2r+1}$ . Define  $L' := L \times \{0, 1\}$  and  $U' := U \times \{0, 1\} \subseteq \{0, 1\}^{2r+1}$ . Then the pair  $(L', U')$  is (balanced) biindependent in  $Q_{2r+1}$ , with  $|L'| = |U'| = a(2r) = \frac{1}{2}a(2r + 1)$ , which implies  $h_{\text{bi}}(Q_{2r+1}) \geq \frac{1}{4}a(2r + 1)$ .

The above construction can be used to show that  $\alpha_{\text{bal}}(Q_r) \geq a(r - 1)$  for all  $r \geq 1$ . For this, given  $A \subseteq \{0, 1\}^r$ , define the following subsets of  $\{0, 1\}^{r+1}$  obtained by adding a parity bit,

$$A_{\text{even}} := \{(x, |x| \bmod 2) : x \in A\} \subseteq \{0, 1\}^{r+1},$$

$$A_{\text{odd}} := \{(x, |x| + 1 \bmod 2) : x \in A\} \subseteq \{0, 1\}^{r+1}.$$

Applying this to the above sets  $L, U \subseteq \{0, 1\}^{2r}$ , we obtain  $L_{\text{even}}, U_{\text{odd}} \subseteq \{0, 1\}^{2r+1}$  such that  $(L_{\text{even}}, U_{\text{odd}})$  is balanced bipartite biindependent in  $Q_{2r+1}$  with  $|L_{\text{even}}| = |U_{\text{odd}}| = |L| = a(2r)/2$ , which implies  $\alpha_{\text{bal}}(Q_{2r+1}) \geq a(2r)$ . Similarly, using the sets  $L', U' \subseteq \{0, 1\}^{2r+1}$ , we obtain  $L'_{\text{even}}, U'_{\text{odd}} \subseteq \{0, 1\}^{2r+2}$  that provide a balanced bipartite biindependent pair in  $Q_{2r+2}$  with

$$|L'_{\text{even}}| = |U'_{\text{odd}}| = |L'| = a(2r + 1)/2,$$

which implies  $\alpha_{\text{bal}}(Q_{2r+2}) \geq a(2r + 1)$ .

**Conjecture 7.29.** *We conjecture that equality  $\alpha_{\text{bal}}(Q_r) = a(r - 1)$  holds for all  $r \geq 1$ .*

We have verified numerically that Conjecture 7.29 indeed holds for any  $r \leq 13$ . For  $r \leq 8$  this can be verified using an integer programming solver (like Gurobi [Gur]). For larger values  $r \leq 13$  we show this in an indirect manner. We consider the semidefinite upper bound on  $\alpha_{\text{bal}}(Q_r)$  that is obtained from the Lasserre relaxation of order 2. After applying a symmetry reduction (as done in [GMS12, LPS17]), we solve the resulting semidefinite program numerically and obtain an upper bound that coincides with  $a(r - 1)$  for  $r \leq 13$ . In addition,  $\alpha_{\text{bal}}(Q_r)/a(r - 1) \rightarrow 1$  as  $r \rightarrow \infty$  since  $\alpha_{\text{bal}}(Q_r) \leq \alpha(Q_r) = 2^{r-1}$  and  $a(r - 1) \sim 2^{r-1}$ .

Observe that  $\alpha_{\text{bal}}(Q_{r+1}) \geq 2 \cdot \alpha_{\text{bal}}(Q_r)$ . For this, for  $x \in \{0, 1\}^r$  let  $x' \in \{0, 1\}^r$  be obtained by switching the last bit of  $x$ , so that the weights of  $x, x'$  have distinct parities and, for a set  $A \subseteq \{0, 1\}^r$  and  $b \in \{0, 1\}$ , define  $Ab := \{(x, b) : x \in A\} \subseteq \{0, 1\}^{r+1}$ . The claim now follows from the fact that if  $(A, B)$  is a balanced bipartite biindependent pair in  $Q_r$ , then the pair  $(B1 \cup B'0, A1 \cup A'0)$  is balanced bipartite biindependent in  $Q_{r+1}$  with size  $2|A \cup B|$ . Hence, the above conjecture implies equality  $\alpha_{\text{bal}}(Q_{r+1}) = 2 \cdot \alpha_{\text{bal}}(Q_r)$  for  $r$  odd.

Interestingly, the sequence  $a(r)$  in (7.58) corresponds to the sequence A307768 in OEIS [OESIS], which counts the number of heads-or-tails games

of length  $r$  during which at some point there are as many heads as tails. It is also related to several other well-known combinatorial counting problems; see, e.g., [EK99] or [Fel57, Chapter III] for an overview. It would be interesting to understand the exact relationship of this sequence with the parameter  $\alpha_{\text{bal}}(Q_r)$ .

### 7.6. Lasserre bounds for the balanced parameters

In this section we turn our attention to the “balanced” parameters  $\alpha_{\text{bal}}(G)$ ,  $g_{\text{bal}}(G)$  and  $h_{\text{bal}}(G)$  that are obtained by restricting the optimization to balanced bipartite biindependent pairs in the definition of  $\alpha(G)$ ,  $g(G)$  and  $h(G)$ . Recall from (7.3) that  $\frac{1}{4}\alpha_{\text{bal}}(G) = \frac{1}{2}\sqrt{g_{\text{bal}}(G)} = h_{\text{bal}}(G)$ . Since these are NP-hard parameters one is interested in finding efficient bounds for them, strengthening those for the original parameters  $g(G)$  and  $h(G)$ .

Let  $G = (V = V_1 \cup V_2, E)$  be a bipartite graph. Following the approach in Section 1.5, each of the parameters  $\alpha_{\text{bal}}(G)$ ,  $g_{\text{bal}}(G)$  and  $h_{\text{bal}}(G)$  has a natural polynomial optimization formulation, which offers the starting point to define several hierarchies of semidefinite relaxations. For this define the vector

$$f := \chi^{V_1} - \chi^{V_2}.$$

Let  $I_{G,\text{bal}}$  denote the ideal in  $\mathbb{R}[x]$  that is generated by the ideal  $I_G$  (itself generated by  $x_i^2 - x_i$  for  $i \in V$  and  $x_i x_j$  for  $\{i, j\} \in E$ ) and the polynomial  $f^\top x$ . For an integer  $t$  let  $I_{G,\text{bal},t}$  denote its truncation at degree  $t$ , where all summands are restricted to have degree at most  $t$ . Then, the formulation for  $\alpha_{\text{bal}}(G)$  follows by replacing the ideal  $I_G$  by the ideal  $I_{G,\text{bal}}$  in (3.4). Similarly,  $g_{\text{bal}}(G)$  (resp.,  $h_{\text{bal}}(G)$ ) is obtained by adding the “balancing” constraint  $f^\top x = 0$  to the program (7.22) defining  $g(G)$  (resp., to the program (7.23) defining  $h(G)$ ). Now, each of these polynomial optimization formulations can be used to define a Lasserre-type hierarchy. In this way one obtains the hierarchies  $\text{las}_{\text{bal},r}(G)$ ,  $g_{\text{bal},r}(G)$ , and  $h_{\text{bal},r}(G)$  for  $r \in \mathbb{N}$  that converge to  $\alpha_{\text{bal}}(G)$ ,  $g_{\text{bal}}(G)$ , and  $h_{\text{bal}}(G)$ , respectively, after  $r \geq \alpha(G)$  steps. They are obtained, respectively, from the programs (3.7) (defining  $\text{las}_r(G)$ ), (7.24) (defining  $g_r(G)$ ), and (7.25) (defining  $h_r(G)$ ) by replacing the truncated ideal  $I_{G,2r}$  by its balanced analog  $I_{G,\text{bal},2r}$ ; that is,

$$\begin{aligned} \text{las}_{\text{bal},r}(G) &= \min \{ \lambda : \lambda - x^\top x \in \Sigma_{2r} + I_{G,\text{bal},2r} \}, \\ g_{\text{bal},r}(G) &= \min \{ \lambda : \lambda - x^\top Cx \in \Sigma_{2r} + I_{G,\text{bal},2r} \}, \\ h_{\text{bal},r} &= \min \{ \lambda : x^\top (\lambda I - C)x \in \Sigma_{2r} + I_{G,\text{bal},2r} \}. \end{aligned}$$

We will now focus on the Lasserre bounds of order  $r = 1$ . We will give explicit semidefinite formulations and show relationships between the various parameters. The parameter  $\text{las}_{\text{bal},1}(G)$  is the analog of  $\text{las}_1(G) = \vartheta(G)$  obtained by adding a balancing constraint to program (7.20). However, adding a balancing constraint to the formulation of  $\vartheta(G)$  in (3.1) leads to another parameter  $\vartheta_{\text{bal}}(G)$  that is in general weaker than  $\text{las}_{\text{bal},1}(G)$ . The parameters

$g_{\text{bal},1}(G)$  and  $h_{\text{bal},1}(G)$  are obtained by adding a balancing constraint to the respective programs defining  $g_1(G)$  and  $h_1(G)$ . Moreover, they can be shown to be nested between  $\text{las}_{\text{bal},1}(G)$  and  $\vartheta_{\text{bal}}(G)$ , see Proposition 7.33 below. For bipartite regular graphs we will investigate some natural symmetric variations of these parameters, with the hope of obtaining a new closed-form parameter strengthening  $\widehat{h}(G)$ . However, as we will show, it turns out that in all cases one recovers the parameter  $\widehat{h}(G)$ , see Propositions 7.36 and 7.37. So the refined formulations taking into account the balancing constraints do not yet lead to stronger eigenvalue bounds for the parameter  $\alpha_{\text{bal}}(\cdot)$ .

**7.6.1. The Lasserre bounds of order  $r = 1$  for the balanced parameters.** We begin with semidefinite reformulations for the parameter  $\text{las}_{\text{bal},1}(G)$ .

**Lemma 7.30.** *For any bipartite graph  $G = (V, E)$  we have*

$$\text{las}_{\text{bal},1}(G) = \max_{X \in \mathcal{S}^{|V|}} \left\{ \langle I, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^{\top} \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, X_{ij} = 0 \text{ if } \{i, j\} \in E, \right. \\ \left. \langle f f^{\top}, X \rangle = 0 \right\}, \tag{7.59}$$

$$= \min_{Z \in \mathcal{S}^{|V|}, u \in \mathbb{R}^{|V|}, s \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -u^{\top}/2 \\ -u/2 & \text{Diag}(u) - I + Z + s f f^{\top} \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}. \tag{7.60}$$

PROOF. As in Section 7.3.1 the proof uses Lemma 7.15. By definition,  $\text{las}_{\text{bal},1}(G)$  is the smallest scalar  $\lambda$  for which  $\lambda - x^{\top} I x \in \Sigma_2 + I_{G,\text{bal},2}$ , i.e.,  $\lambda - x^{\top} I x - (a_0 + a^{\top} x) f^{\top} x \in \Sigma_2 + I_{G,2}$  for some  $a_0 \in \mathbb{R}$ ,  $a \in \mathbb{R}^n$ . Thus,  $\text{las}_{\text{bal},1}(G)$  is the smallest  $\lambda$  such that  $[x]_1^{\top} \left( Q - \begin{pmatrix} \lambda & a_0 f^{\top}/2 \\ a_0 f/2 & -I + \frac{a f^{\top} + f a^{\top}}{2} \end{pmatrix} \right) [x]_1 \in I_{G,2}$  for some  $a_0 \in \mathbb{R}$ ,  $a \in \mathbb{R}^n$ . Applying Lemma 7.15 we arrive at the program

$$\text{las}_{\text{bal},1}(G) = \min_{\substack{Z \in \mathcal{S}^{|V|}, \\ u, a \in \mathbb{R}^{|V|}, \\ a_0 \in \mathbb{R}}} \left\{ \lambda : \begin{pmatrix} \lambda & \frac{1}{2}(-u + a_0 f)^{\top} \\ \frac{1}{2}(-u + a_0 f) & \text{Diag}(u) - I + Z + \frac{a f^{\top} + f a^{\top}}{2} \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}.$$

Now, we take the dual of this semidefinite program. We also apply some simplifications, such as observing that  $X f = 0$  is equivalent to  $\langle f f^{\top}, X \rangle = 0$  when  $X \succeq 0$ , which in turn implies  $f^{\top} \text{diag}(X) = 0$  when  $\begin{pmatrix} 1 & \text{diag}(X)^{\top} \\ \text{diag}(X) & X \end{pmatrix}$  is positive semidefinite. In this way we arrive at the program (7.59). Taking the dual of (7.59) gives the (simplified) program (7.60). Note that strong duality holds since program (7.60) is strictly feasible (e.g., take  $s = 0$ ,  $Z = 0$ ,  $u = \mu e$  with  $\mu > 1$ , and  $\lambda > \frac{n}{4} \frac{\mu^2}{\mu - 1}$ ).  $\square$

Hence, program (7.59) is the analog of program (7.20) defining  $\text{las}_1(G) = \vartheta(G)$  to which we add the balancing condition  $\langle f f^{\top}, X \rangle = 0$ . Next we consider the analog of program (3.1) to which we add the balancing conditions

$\langle ff^\top, X \rangle = 0$  and  $f^\top \text{diag}(X) = 0$ , giving the parameter

$$\vartheta_{\text{bal}}(G) := \max_{X \in \mathcal{S}^{|V|}} \{ \langle J, X \rangle : X \succeq 0, \text{Tr}(X) = 1, X_{ij} = 0 \text{ if } \{i, j\} \in E, \langle ff^\top, X \rangle = 0, \langle \text{Diag}(f), X \rangle = 0 \}, \tag{7.61}$$

$$= \min_{Z \in \mathcal{S}^{|V|}, \lambda, s, v \in \mathbb{R}} \left\{ \lambda : \lambda I - J + Z + v \text{Diag}(f) + sff^\top \succeq 0, Z \in \mathcal{S}_G \right\}, \tag{7.62}$$

where the second formulation (7.62) follows by taking the dual of (7.61) (and observing that (7.62) is strictly feasible). We will see in Proposition 7.33 below that  $\vartheta_{\text{bal}}(G)$  provides a weaker bound for  $\alpha_{\text{bal}}(G)$  than  $\text{las}_{\text{bal},1}(G)$ .

We now consider the parameter  $g_{\text{bal},1}(G)$ . By definition,  $g_{\text{bal},1}(G)$  is the smallest scalar  $\lambda$  for which  $\lambda - x^\top Cx \in \Sigma_2 + I_{G,\text{bal},2}$ . Comparing with the definition of  $\text{las}_{\text{bal},1}(G)$ , we see that it suffices to exchange the matrices  $C$  and  $I$  to get the semidefinite formulations of  $g_{\text{bal},1}(G)$  in the next lemma (recall also Remark 7.18).

**Lemma 7.31.** *For any bipartite graph  $G = (V, E)$  we have*

$$g_{\text{bal},1}(G) = \max_{X \in \mathcal{S}^{|V|}} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & \text{diag}(X)^\top \\ \text{diag}(X) & X \end{pmatrix} \succeq 0, X_{ij} = 0 \text{ if } \{i, j\} \in E, \langle ff^\top, X \rangle = 0 \right\}, \tag{7.63}$$

$$= \min_{\lambda, s \in \mathbb{R}, u \in \mathbb{R}^{|V|}, Z \in \mathcal{S}^{|V|}} \left\{ \lambda : \begin{pmatrix} \lambda & -u^\top/2 \\ -u/2 & \text{Diag}(u) - C + Z + sff^\top \end{pmatrix} \succeq 0, Z \in \mathcal{S}_G \right\}. \tag{7.64}$$

Finally we give semidefinite formulations for the parameter  $h_{\text{bal},1}(G)$ .

**Lemma 7.32.** *Let  $G = (V, E)$  be a bipartite graph. Then we have*

$$h_{\text{bal},1}(G) = \max_{X \in \mathcal{S}^{|V|}} \{ \langle C, X \rangle : X \succeq 0, \text{Tr}(X) = 1, X_{ij} = 0 \text{ if } \{i, j\} \in E, \langle ff^\top, X \rangle = 0, \langle \text{Diag}(f), X \rangle = 0 \}, \tag{7.65}$$

$$h_{\text{bal},1}(G) = \min_{\lambda, v, s \in \mathbb{R}, Z \in \mathcal{S}^{|V|}} \{ \lambda : \lambda I - C + Z + v \text{Diag}(f) + sff^\top \succeq 0, Z \in \mathcal{S}_G \}. \tag{7.66}$$

PROOF. The argument is similar to the one used to show Lemma 7.30. Namely, one starts with the definition of  $h_{\text{bal},1}(G)$  as the smallest  $\lambda$  for which  $x^\top(\lambda I - C)x \in \Sigma_2 + I_{G,\text{bal},2}$ . Using Lemma 7.15 one arrives at a semidefinite program whose dual can be shown (after some simplifications) to take the form (7.65). Then one takes the dual of program (7.65), which has the form (7.66).  $\square$

We now compare the parameters  $\text{las}_{\text{bal},1}(G)$ ,  $\vartheta_{\text{bal}}(G)$ ,  $g_{\text{bal},1}(G)$  and  $h_{\text{bal},1}(G)$ .

**Proposition 7.33.** *For any bipartite graph  $G$ , we have the inequalities*

$$\frac{1}{4} \text{las}_{\text{bal},1}(G) \leq \frac{1}{2} \sqrt{g_{\text{bal},1}(G)} \leq h_{\text{bal},1}(G) = \frac{1}{4} \vartheta_{\text{bal}}(G).$$

Moreover, we have  $\frac{1}{2} \sqrt{g_{\text{bal},1}(G)} = \frac{1}{4} \vartheta_{\text{bal}}(G) \iff \text{las}_{\text{bal},1}(G) = \vartheta_{\text{bal}}(G)$ .

PROOF. The equality  $\vartheta_{\text{bal}}(G) = 4h_{\text{bal},1}(G)$  follows from the fact that the programs (7.61) (defining  $\vartheta_{\text{bal}}(G)$ ) and (7.65) (defining  $h_{\text{bal},1}(G)$ ) differ only in their objective functions that are, respectively,  $\langle J, X \rangle$  and  $\langle C, X \rangle$ , combined with the identity  $J - 4C = ff^T$ .

The inequality  $\text{las}_{\text{bal},1}(G) \leq \vartheta_{\text{bal}}(G)$  follows using the formulations (7.59) and (7.61) and a classic argument (repeated for convenience). If  $X$  is optimal for (7.59) with  $x := \text{diag}(X)$ , then  $X - xx^T \succeq 0$ ,  $f^T x = 0$ ,  $\text{Tr}(X) = e^T x$ , so  $X/\text{Tr}(X) = X/e^T x$  is feasible for (7.61) and thus we have  $\vartheta_{\text{bal}}(G) \geq \frac{1}{e^T x} \langle J, X \rangle \geq \frac{1}{e^T x} \langle J, xx^T \rangle = e^T x = \text{las}_{\text{bal},1}(G)$ .

For the inequality  $\text{las}_{\text{bal},1}(G)^2 \leq 4 \cdot g_{\text{bal},1}(G)$ , pick an optimal solution  $X$  for (7.59) with  $x := \text{diag}(X)$ , so that  $X - xx^T \succeq 0$ , and use again the fact that  $4C = J - ff^T$ . Then we have  $4 \cdot g_{\text{bal},1}(G) \geq \langle 4C, X \rangle = \langle J, X \rangle \geq \langle J, xx^T \rangle = (e^T x)^2 = \langle I, X \rangle^2 = \text{las}_{\text{bal},1}(G)^2$ .

We now show the inequality  $4 \cdot g_{\text{bal},1}(G) \leq \vartheta_{\text{bal}}(G)^2$ . For this let  $X$  be optimal for program (7.63) defining  $g_{\text{bal},1}(G)$ . Then  $X$  is feasible for (7.59) and thus  $\text{las}_{\text{bal},1}(G) \geq \text{Tr}(X)$ . In addition,  $X/\text{Tr}(X)$  is feasible for (7.61) and thus  $\vartheta_{\text{bal}}(G) \geq \frac{1}{\text{Tr}(X)} \langle J, X \rangle$ . Using  $4C = J - ff^T$ , we obtain  $4 \cdot g_{\text{bal},1}(G) = \langle 4C, X \rangle = \langle J, X \rangle = \text{Tr}(X) \cdot \langle J, X/\text{Tr}(X) \rangle \leq \text{las}_{\text{bal},1}(G) \cdot \vartheta_{\text{bal}}(G) \leq \vartheta_{\text{bal}}(G)^2$ . Finally, this argument also shows that equality  $4 \cdot g_{\text{bal},1}(G) = \vartheta_{\text{bal}}(G)^2$  implies  $\text{las}_{\text{bal},1}(G) = \vartheta_{\text{bal}}(G)$ , which concludes the proof.  $\square$

Quite surprisingly, while we had the inequality  $h_1(G) \leq \frac{1}{2} \sqrt{g_1(G)}$  (recall Proposition 7.2), we now have the reverse inequality  $\frac{1}{2} \sqrt{g_{\text{bal},1}(G)} \leq h_{\text{bal},1}(G)$  for the balanced analogs. We next give an example where this inequality is strict.

**Example 7.34.** *Let  $G$  be the bipartite graph from Figure 7.4. One can check that  $h_{\text{bal},1}(G) = 2/3$ ,  $g_{\text{bal},1}(G) = 4/3$  and  $\text{las}_{\text{bal},1}(G) = 9/4$ , which shows that the strict inequalities  $\frac{1}{4} \text{las}_{\text{bal},1}(G) < \frac{1}{2} \sqrt{g_{\text{bal},1}(G)} < h_{\text{bal},1}(G)$  hold. To see this, consider the matrices*

$$X_1 = \frac{1}{12} \begin{pmatrix} 1 & 1 & 0 & 2 \\ 1 & 5 & 2 & 4 \\ 0 & 2 & 1 & 1 \\ 2 & 4 & 1 & 5 \end{pmatrix}, \quad X_2 = \frac{1}{9} \begin{pmatrix} 3 & 1 & 0 & 4 \\ 1 & 7 & 4 & 4 \\ 0 & 4 & 3 & 1 \\ 4 & 4 & 1 & 7 \end{pmatrix}, \quad X_3 = \frac{1}{32} \begin{pmatrix} 12 & 3 & 0 & 15 \\ 3 & 24 & 15 & 12 \\ 0 & 15 & 12 & 3 \\ 15 & 12 & 3 & 24 \end{pmatrix}.$$

Then,  $X_1$  is feasible for (7.65) with  $\langle C, X_1 \rangle = 2/3$ ,  $X_2$  is feasible for (7.63) with  $\langle C, X_2 \rangle = 4/3$ , and  $X_3$  is feasible for (7.59) with  $\langle I, X_3 \rangle = 9/4$ . One can check optimality of these solutions for the respective programs (for this, use the constraint  $\langle ff^T, X \rangle = 0$  to reduce the semidefinite program to an equivalent semidefinite program involving smaller matrices, and then construct a solution of the dual program with the same objective value).

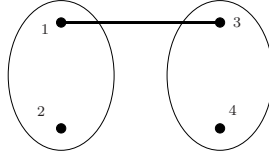


FIGURE 7.4. Graph  $G$  with  $\alpha(G) = 3$ ,  $\alpha_{\text{bal}}(G) = 2$ ,  $h(G) = 2/3$ , and  $g(G) = 2$

**7.6.2. Symmetric versions of the parameters**  $\text{las}_{\text{bal},1}(G)$ ,  $\vartheta_{\text{bal}}(G)$  and  $g_{\text{bal},1}(G)$ . Here, we address the question whether it is possible to obtain closed-form eigenvalue-based upper bounds for  $\alpha_{\text{bal}}(G)$  that improve on the spectral parameter  $\widehat{h}(G)$  from (7.42). For this, a natural approach is to restrict the optimization in the programs (7.60), (7.62), (7.64) to matrices  $Z = tA_G$  for some  $t \in \mathbb{R}$  and, for (7.60) and (7.64), to vectors  $u = \mu e$  for some  $\mu \in \mathbb{R}$ . Moreover, we add a term  $v\text{Diag}(f)$  to the matrix involved in (7.60) and (7.64), which amounts to adding the redundant constraint  $\langle \text{Diag}(f), X \rangle = 0$  to the programs (7.59) and (7.63). The motivation for this is to get possibly sharper bounds. In addition, the bounds obtained in this way are easier to compare (see Proposition 7.35). However, as we will show in Proposition 7.36, these additional constraints will turn out to be redundant for bipartite regular graphs.

So we consider the parameters

$$\begin{aligned} \widehat{\text{las}}_{\text{bal}}(G) &:= \min_{\lambda, \mu, t, s, v \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -\mu e^\top / 2 \\ -\mu e / 2 & (\mu - 1)I + tA_G + sff^\top + v\text{Diag}(f) \end{pmatrix} \succeq 0 \right\}, \\ &= \max_{X \in \mathcal{S}^V, x \in \mathbb{R}^V} \left\{ \langle I, X \rangle : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0, \text{Tr}(X) = e^\top x, \langle A_G, X \rangle = 0, \right. \\ &\quad \left. \langle ff^\top, X \rangle = 0, \langle \text{Diag}(f), X \rangle = 0 \right\}, \end{aligned} \tag{7.67}$$

(7.68)



$$\widehat{\vartheta}_{\text{bal}}(G) := \min_{\lambda, t, v, s \in \mathbb{R}} \{ \lambda : \lambda I - J + tA_G + v\text{Diag}(f) + sff^\top \succeq 0 \}, \quad (7.69)$$

$$= \max \{ \langle J, X \rangle : X \succeq 0, \text{Tr}(X) = 1, \langle A_G, X \rangle = 0, \langle ff^\top, X \rangle = 0, \langle \text{Diag}(f), X \rangle = 0 \}, \quad (7.70)$$

$$\widehat{g}_{\text{bal}}(G) := \min_{\lambda, \mu, t, s, v \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & & & -\mu e^\top / 2 \\ & \mu I - C + tA_G + sff^\top + v\text{Diag}(f) & & \\ & & & \end{pmatrix} \succeq 0 \right\}, \quad (7.71)$$

$$= \max_{X \in \mathcal{S}^V, x \in \mathbb{R}^V} \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0, \text{Tr}(X) = e^\top x, \langle X, A_G \rangle = 0, \right.$$

$$\left. \langle ff^\top, X \rangle = 0, \langle \text{Diag}(f), X \rangle = 0 \right\}.$$

(Since each of the programs (7.67), (7.69), (7.71) is strictly feasible, strong duality holds as claimed above.) We begin with comparing the above parameters and show the analog of Proposition 7.33.

**Proposition 7.35.** *For any bipartite graph  $G$ , we have*

$$\frac{1}{4} \widehat{\text{las}}_{\text{bal}}(G) \leq \frac{1}{2} \sqrt{\widehat{g}_{\text{bal}}(G)} \leq \frac{1}{4} \widehat{\vartheta}_{\text{bal}}(G).$$

PROOF. We use the formulations (7.68), (7.70), (7.72) for the parameters  $\widehat{\text{las}}_{\text{bal}}(G)$ ,  $\widehat{\vartheta}_{\text{bal}}(G)$ ,  $\widehat{g}_{\text{bal}}(G)$ , respectively. Then, the inequalities follow in the same way as in the proof of Proposition 7.33.  $\square$

Next we compute the parameter  $\widehat{\vartheta}_{\text{bal}}(G)$  and show its relation to  $\widehat{h}(G)$ .

**Proposition 7.36.** *Assume  $G = (V_1 \cup V_2, E)$  is bipartite  $r$ -regular, set  $n := |V_1| = |V_2|$  and let  $\lambda_2$  denote the second largest eigenvalue of  $A_G$ . Then we have  $\widehat{\vartheta}_{\text{bal}}(G) = \frac{2n\lambda_2}{r+\lambda_2} = 4 \cdot \widehat{h}(G)$ .*

We omit the proof in this thesis, which is a bit technical. A full proof of this result can be found in my work [LPV23, Appendix D] with Laurent and Polak. As the proof shows, the program (7.69) defining  $\widehat{\vartheta}_{\text{bal}}(G)$  admits an optimal solution with  $v = 0$ . Hence, when  $G$  is bipartite regular, the constraint  $\langle \text{Diag}(f), X \rangle = 0$  is redundant in program (7.69) and one can set  $v = 0$  in program (7.69), and the same observation applies to the programs defining  $\widehat{g}_{\text{bal}}(G)$  and  $\widehat{\text{las}}_{\text{bal}}(G)$ .

We can now compute the parameters  $\widehat{\text{las}}_{\text{bal}}(G)$  and  $\widehat{g}_{\text{bal}}(G)$  and show their relation to  $\widehat{h}(G)$ .

**Proposition 7.37.** *For any regular bipartite graph  $G$  we have*

$$\frac{1}{4}\widehat{\text{las}}_{\text{bal}}(G) = \frac{1}{2}\sqrt{\widehat{g}_{\text{bal}}(G)} = \frac{1}{4}\widehat{\vartheta}_{\text{bal}}(G) = \widehat{h}(G).$$

PROOF. Assume  $G$  is bipartite regular and set  $n := |V_1| = |V_2|$ . If  $G$  is complete bipartite, then  $\alpha_{\text{bal}}(G) = 0$  and, using (7.70) and Proposition 7.35, one can check that  $\widehat{\vartheta}_{\text{bal}}(G) = 0$ , so the result holds. We now assume that  $G$  is not complete bipartite. In view of Propositions 7.35 and 7.36 it suffices to show  $\widehat{\text{las}}_{\text{bal}}(G) \geq \widehat{\vartheta}_{\text{bal}}(G)$ . Assume that  $(\lambda, \mu, t, s, v)$  is feasible for the program (7.67) defining  $\widehat{\text{las}}_{\text{bal}}(G)$ , we construct a feasible solution for the program (7.69) defining  $\widehat{\vartheta}_{\text{bal}}(G)$  with the same objective value  $\lambda$ . Call  $Q \in \mathcal{S}^{1+|V_1|+|V_2|}$  the matrix appearing in program (7.67). By taking a Schur complement with respect to its upper left corner entry  $\lambda$ , we obtain

$$\lambda((\mu - 1)I + tA_G + sff^\top + v\text{Diag}(f)) - \frac{\mu^2}{4}J \succeq 0.$$

We now claim that  $\mu > 1$ . For this observe that the submatrices of  $Q$  indexed by  $V_1$  and  $V_2$  read  $(\mu - 1)I_n + sJ_n \pm vI_n$ . Since they are both positive semidefinite this implies  $(\mu - 1)I_n + sJ_n \succeq 0$  and thus  $\mu \geq 1$ . Assume that  $\mu = 1$ . Then the conditions  $sJ_n \pm vI_n \succeq 0$  imply  $v = 0$ . Let  $i \in V_1$  and  $j \in V_2$  that are not adjacent (they exist since  $G \neq K_{n,n}$ ). Then the principal submatrix of  $Q$  indexed by  $\{0, i, j\}$  takes the form  $\begin{pmatrix} \lambda & -1/2 & -1/2 \\ -1/2 & s & -s \\ -1/2 & -s & s \end{pmatrix}$  and it must be positive semidefinite, so we reach a contradiction. Hence we have  $\mu > 1$ . Thus we can scale the above matrix and obtain

$$\lambda I + \frac{\lambda t}{\mu - 1}A_G + \frac{\lambda s}{\mu - 1}ff^\top + \frac{\lambda v}{\mu - 1}\text{Diag}(f) - \frac{\mu^2}{4(\mu - 1)}J \succeq 0.$$

Note that  $\frac{\mu^2}{4(\mu - 1)} - 1 = \frac{(\mu - 2)^2}{4(\mu - 1)} \geq 0$  and add  $(\frac{\mu^2}{4(\mu - 1)} - 1)J \succeq 0$  to the above matrix. So we obtain

$$\lambda I + \frac{\lambda t}{\mu - 1}A_G + \frac{\lambda s}{\mu - 1}ff^\top + \frac{\lambda v}{\mu - 1}\text{Diag}(f) - J \succeq 0,$$

which gives a feasible solution to the formulation (7.69) of  $\widehat{\vartheta}_{\text{bal}}(G)$  and thus shows  $\widehat{\vartheta}_{\text{bal}}(G) \leq \lambda = \widehat{\text{las}}_{\text{bal}}(G)$ .  $\square$

**Acknowledgements.** We are grateful to Aida Abiad for discussions and bringing the paper [CK03] to our attention.

## Concluding remarks

In this thesis, we studied sum-of-squares representations for polynomials arising from copositive matrices and independent (and biindependent) sets in graphs. In this chapter, we briefly summarize the main results of the thesis and highlight open questions and possible directions for future research.

### Copositive matrices and the cones $\mathcal{K}_n^{(r)}$

One of the main results of this thesis is a characterization of the matrix sizes  $n$  for which the cones  $\mathcal{K}_n^{(r)}$  cover the full copositive cone  $\text{COP}_n$ . Namely, we have the equality

$$\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} = \text{COP}_n \text{ for } n \leq 5$$

(see Theorem 2.2), and we have that the inclusion

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

is strict for  $n \geq 6$ . Another interesting case of study is when restricting to copositive matrices with an all-ones diagonal. It was shown in [DDGH13] that every  $5 \times 5$  copositive matrix with an all-ones diagonal belongs to the cone  $\mathcal{K}_n^{(1)}$ . In Chapter 2, we found examples of copositive matrices with an all-ones diagonal of size  $n \times n$  (for any  $n \geq 7$ ) that do not belong to any cone  $\mathcal{K}_n^{(r)}$ . The case  $n = 6$  remains open.

**Question 8.1.** *Does every  $6 \times 6$  copositive matrix with an all-ones diagonal belong to  $\bigcup_{r \geq 0} \mathcal{K}_6^{(r)}$ ?*

Recently, Hildebrand and Afonin [HA22] gave an example of a  $6 \times 6$  copositive matrix with an all-ones diagonal that does not belong to the cone  $\mathcal{K}_6^{(1)}$ , showing that the result for matrix size  $n = 5$  does not extend to  $n = 6$ . It is even open whether there exists a fixed  $r \in \mathbb{N}$  for which  $\mathcal{K}_6^{(r)}$  contains all those matrices.

**Question 8.2.** *Does there exist an integer  $r \in \mathbb{N}$  such that every  $6 \times 6$  copositive matrix with an all-ones diagonal belongs to  $\mathcal{K}_6^{(r)}$ ?*

**Graph matrices  $M_G$ , cones  $\mathcal{K}_n^{(r)}$ ,  $\text{LAS}_{\Delta_n}^{(r)}$  and  $\mathcal{Q}_n^{(r)}$**

Another main result of this thesis is showing that, for every graph  $G$ , the graph matrix  $M_G$  belongs to  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ , see Theorem 3.8. This result is equivalent to the finite convergence of the hierarchy  $\vartheta^{(r)}(G)$  to  $\alpha(G)$ . In other words, the parameter  $\vartheta\text{-rank}(G)$  is always finite. However, we did not obtain any bound on the degree  $r$  of the convergence. We recall the conjecture proposed by de Klerk and Pasechnik [dKP02] (Conjecture 3.7), which remains open:

**Conjecture 8.3** ([dKP02]). *For any graph  $G$ , we have  $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$ , i.e.,  $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$ .*

Observe that, unless  $\text{P}=\text{NP}$ , there is no constant  $r \in \mathbb{N}$  such that  $\vartheta\text{-rank}(G) \leq r$  for all graphs  $G$ , otherwise  $\alpha(G)$  could be found by computing (with accuracy  $\frac{1}{4}$ ) the bound  $\vartheta^{(r)}(G)$ , which can be done in polynomial time as  $r$  is constant. However, we do not know specific graphs with large  $\vartheta\text{-rank}$ . Specifically, the following problem is open.

**Problem 8.4.** *Given an integer  $k$ , find a graph  $G$  such that  $\vartheta\text{-rank}(G) \geq k$ .*

We also characterize the graphs  $G$  for which the graph matrix  $M_G$  belongs to  $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ . Namely, they are the graphs obtained by adding twin nodes to acritical graphs. In other words, this is the characterization of graphs for which the simplex-based Lasserre hierarchy  $p_G^{(r)}$  (recall relation (4.1)) converges to  $1/\alpha(G)$  in finitely many steps. We observe that the degree of convergence should be unbounded for acritical graphs. This follows from the fact that computing  $\alpha(G)$  is hard already for acritical graphs (see Theorem 4.28). Similar to the case of the  $\vartheta\text{-rank}$ , we do not have an explicit class of acritical graphs for which the hierarchy  $p_G^{(r)}$  takes an unbounded number of steps for converging to  $1/\alpha(G)$ .

We finish this section with a discussion about the cones  $\mathcal{Q}_n^{(r)}$ . It was shown in [GL07] that Conjecture 8.3 holds for graphs with  $\alpha(G) \leq 8$ , that is,  $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$ . It was observed that the proof of this result extends to the cones  $\mathcal{Q}_n^{(r)}$ , thus  $M_G \in \mathcal{Q}_n^{(\alpha(G)-1)}$  for graphs with  $\alpha(G) \leq 8$ . The question whether the cones  $\mathcal{Q}_n^{(r)}$  satisfy a result as in Conjecture 8.3 (i.e., whether  $M_G \in \mathcal{Q}_n^{(\alpha(G)-1)}$  or  $\nu\text{-rank}(G) \leq \alpha(G) - 1$  for all graphs  $G$ ) remains open. It was shown in Chapter 5 that if this result holds, then it should be tight, as the graphs  $L_k$  satisfy that  $\nu\text{-rank}(L_k) \geq \alpha(L_k) - 1$ .

The difference between the cones  $\mathcal{K}_n^{(r)}$  and  $\mathcal{Q}_n^{(r)}$  has been studied. It was shown by Peña, Vera and Zuluaga [PVZ07] that there are matrices that

belong to  $\mathcal{K}_n^{(2)}$  and do not belong to  $\mathcal{Q}_n^{(2)}$ . However, to the best of our knowledge, no explicit copositive matrices are known lying in the set difference  $\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \setminus \bigcup_{r \geq 0} \mathcal{Q}_n^{(r)}$ .

It is not clear whether the hierarchy  $\nu^{(r)}(G)$  has finite convergence to  $\alpha(G)$ . This is equivalent to the question of whether every graph matrix belongs to  $\bigcup_{r \geq 0} \mathcal{Q}_n^{(r)}$ .

**Question 8.5.** *Does the hierarchy  $\nu^{(r)}(G)$  has finite convergence to  $\alpha(G)$ , i.e.,  $M_G \in \bigcup_{r \geq 0} \mathcal{Q}_n^{(r)}$  for every graph  $G$ ?*

### Constructing nonnegative polynomials that are not sums of squares

We show that certain polynomials do not admit a sum-of-squares representation. Namely, in Theorem 2.7 in Chapter 2, we show examples of homogeneous polynomials arising from copositive matrices that do not admit a Reznick-type certificate as in (1.8). Also, in Theorem 4.17 in Chapter 4 (see also the proof of Theorem 2.18), we show that certain polynomials  $p$  that are nonnegative on the simplex  $\Delta_n$  do not belong to the corresponding quadratic module  $\mathcal{M}(\mathbf{x}) + I_{\Delta_n}$ . For showing this, we exploit the structure of the infinitely many zeros (in  $\Delta_n$ ) of these polynomials.

The comparison between sums of squares and nonnegative polynomials has been studied recently in the context of convex forms. Indeed, it was shown by Blekherman [B112] that there exist convex forms that cannot be written as a sum of squares. Later in 2020, Saunderson [Sau20] found the first explicit example of a convex form that is not a sum of squares. This example is a form of degree 4 in 272 variables. The question about the minimum number of variables for which such an example exists is open. El Bachir [EIK20] showed that every convex form of degree 4 in 4 variables can be written as a sum of squares. The next case of study are forms of degree 4 in 5 variables. Observe that even forms of degree 4 in 5 variables are precisely polynomials of the form  $(x^{\circ 2})^T M x^{\circ 2}$ , where  $M \in \text{COP}_5$ . Since  $\text{COP}_n \neq \mathcal{K}_n^{(0)}$  for  $n \geq 5$ , it would be an interesting starting point to look at the copositive matrices for which the associated polynomial  $(x^{\circ 2})^T M x^{\circ 2}$  is not a sum of squares, i.e.,  $M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)}$ .

### Complexity questions about polynomial optimization

In Chapter 4, two complexity results about polynomial optimization were shown. Namely, it is NP-hard to decide whether a quadratic form has finitely many minimizers, and it is NP-hard to decide whether the Lasserre hierarchy of a standard quadratic program has finite convergence. For showing these results, we use variations of the Motzkin-Straus formulation and we exploit the structure of their minimizers in connection with the critical edges of the graph. The Motzkin-Straus formulation has been used in different settings

for showing complexity results related to optimization problems as shown by Ahmadi and Zhang [AZ2020a, AZ2020b]. It would be interesting to explore more complexity questions using the Motzkin-Straus formulation and its perturbations.

### Parameters in bipartite graphs

In Chapter 7, we consider semidefinite bounds for several parameters in bipartite graphs. In particular, we consider the bound  $h_1(G)$  that satisfies the following relations:

$$h(G) \leq \frac{1}{2}\sqrt{g(G)} \leq h_1(G).$$

We recall the definition of  $h_1(G)$ :

$$h_1(G) = \max_{X \in S^V} \{ \langle C, X \rangle : X \succeq 0, \operatorname{Tr}(X) = 1, X_{ij} = 0 \text{ if } \{i, j\} \in E \}.$$

A natural strengthening of  $h_1(G)$  is obtained by adding one row/column to the matrix variable:

$$h'_1(G) := \max \left\{ \langle C, X \rangle : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succeq 0, \operatorname{Tr}(X) = 1, x = \operatorname{diag}(X), \right. \\ \left. X_{ij} = 0 \text{ for } \{i, j\} \in E \right\}.$$

It can be shown (see [LPV23]) that

$$h(G) \leq h'_1(G) \leq h_1(G).$$

In my work [LPV23] with Monique Laurent and Sven Polak, we consider the parameter  $\widehat{h}'(G)$  obtained from  $h'_1(G)$ , as the analog of  $\widehat{h}(G)$  (obtained from  $h_1(G)$ ), for regular bipartite graphs with the objective of deriving a better closed-form eigenvalue bound for  $h(G)$ . However, we show that these two bounds, in fact, coincide:  $\widehat{h}'(G) = \widehat{h}(G)$ .

In addition, for the parameter  $\alpha_{\text{bal}}(G)$  we also consider semidefinite bounds  $\text{las}_{\text{bal},1}(G)$ ,  $\vartheta_{\text{bal}}(G)$  and  $g_{\text{bal},1}(G)$  and their respective symmetric versions  $\widehat{\text{las}}_{\text{bal}}(G)$ ,  $\widehat{\vartheta}_{\text{bal}}(G)$  and  $\widehat{g}_{\text{bal}}(G)$ . We show that these parameters (up to transformation) coincide with  $\widehat{h}(G)$ :

$$\frac{1}{4}\widehat{\text{las}}_{\text{bal}}(G) = \frac{1}{2}\sqrt{\widehat{g}_{\text{bal}}(G)} = \frac{1}{4}\widehat{\vartheta}_{\text{bal}}(G) = \widehat{h}(G).$$

One idea for trying to get a stronger closed-form bound for  $\alpha_{\text{bal}}(G)$  could be to consider a possibly weaker symmetrization of the parameter  $\text{las}_{\text{bal},1}(G)$ , where we now allow a vector  $u$  taking distinct values for nodes in  $V_1$  and in  $V_2$  instead of restricting to  $u = \mu e$  for some  $\mu \in \mathbb{R}$  (as it was done in formulation

of  $\widehat{\text{las}}_{\text{bal}}(G)$  in (7.67)). So, we consider the following variation  $\widetilde{\text{las}}_{\text{bal}}(G)$  of the parameter  $\widehat{\text{las}}_{\text{bal}}(G)$ , defined by

$$\min_{\lambda, \mu_1, \mu_2, t, s, v \in \mathbb{R}} \left\{ \lambda : \begin{pmatrix} \lambda & -u^\top/2 \\ -u/2 & \text{Diag}(u) - I + tA_G + sff^\top + v\text{Diag}(f) \end{pmatrix} \succeq 0, \right. \\ \left. u = \mu_1\chi^{V_1} + \mu_2\chi^{V_2} \right\}.$$

By its definition, the parameter  $\widetilde{\text{las}}_{\text{bal}}(G)$  lower bounds  $\widehat{\text{las}}_{\text{bal}}(G)$ , for which the optimization is restricted to the case  $\mu_1 = \mu_2$ . It turns out that the two parameters are in fact equal, as we show in [LPV23].

We finish by recalling a conjecture about the balanced parameters for the hypercube graph  $Q_r$ . Recall that the sequence  $a(r)$  is defined as

$$a(2r) = 2^{2r} - \binom{2r}{r}, \quad a(2r + 1) = 2 \cdot a(2r) \text{ if } r \geq 1, \text{ and } a(0) = 0.$$

We have the following conjecture.

**Conjecture 8.6.** *The equality  $\alpha_{\text{bal}}(Q_r) = a(r - 1)$  holds for all  $r \geq 1$ .*

We show that  $\alpha_{\text{bal}}(Q_r) \geq a(r - 1)$  for any  $r \geq 0$ . Computational experiments suggest that this inequality is tight. The sequence  $a(r)$  counts the number of heads-or-tails games of length  $r$  during which at some point there are as many heads as tails. This sequence is also related to several other well-known combinatorial counting problems; see, e.g., [EK99] or [Fel57] for an overview. It would be interesting to understand the relationship of this sequence with the parameter  $\alpha_{\text{bal}}(Q_r)$ .





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## List of symbols

### Graph theory

$G = (V, E)$	Graph with vertex set $V$ and edge set $E$ .
$\alpha(G)$	The stability number of $G$ .
$\chi(G)$	Chromatic number of $G$ .
$\bar{\chi}(G)$	The clique covering number of $G$ .
$N_G(i)$	Neighbors of $i$ in $G$ .
$N_S(i)$	Neighbors of $i$ in $S$ .
$N_G(S)$	Neighbors of the elements of $S$ in $G$ .
$i^\perp$	Extended neighbourhood of $i$ : $N_G(i) \cup \{i\}$ .
$S^\perp$	Extended neighbourhood of $S$ : $N_G(S) \cup S$ .
$G \oplus H$	Disjoint union of the graphs $G$ and $H$ .
$G \oplus i$	Graph obtained by adding the isolated node $i$ to $G$ .

### Polynomials

$\mathbb{R}[x]$	Multivariate polynomials
$\mathbb{R}[x]_r$	Polynomials of degree at most $r$
$[x]_r$	Monomials of degree at most $r$

### Matrices

$\mathcal{S}^n$	Set of $n \times n$ symmetric matrices.
$\mathcal{S}_+^n$	Cone of $n \times n$ positive semidefinite matrices.
$\text{COP}_n$	Cone of $n \times n$ copositive matrices.
$\mathcal{S}_G$	Set of symmetric matrices supported on the graph $G$ .
$I_n$	$n \times n$ identity matrix.
$J_n$	$n \times n$ all-ones matrix.
$\mathcal{D}_+$	Cone of nonnegative diagonal matrices.
$\mathcal{D}_{++}$	Set of positive diagonal matrices.

### special sets

$\Delta_n$	The standard simplex $\{x \in \mathbb{R}^n : \sum_{i=1}^n x_i = 1, x \geq 0\}$ .
$\mathbb{S}^{n-1}$	The unit sphere $\{x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 = 1\}$ .

### Special polynomials and matrices

$M_G$	Matrix $\alpha(G)(A_G + I) - J$ (called the graph matrix of $G$ ).
$H$	Horn matrix.
$p_M$	Quadratic polynomial $x^\top Mx$ .
$p_M^{(r)}$	Simplex-based Lasserre hierarchy for $p_M$ .
$p_G$	When $G$ is a graph, corresponds to the polynomial $p_{A_G+I}$ .
$p_G^{(r)}$	Simplex-based Lasserre hierarchy for $p_{A_G+I}^{(r)}$ .
$f_G$	Quartic polynomial $(x^{\circ 2})^\top M_G x^{\circ 2}$ .

### Polynomial optimization and sums of squares

$\mathbf{g}, \mathbf{h}$	Sets of polynomials $\{g_1, \dots, g_m\}$ and $\{h_1, \dots, h_l\}$ .
$K$	Semialgebraic set.
$f$	Objective polynomial, to be minimized on $K$ .
$f^*$	Optimal value of the polynomial optimization problem.
$\Sigma$	Sums of squares of polynomials.
$\Sigma_r$	$\Sigma \cap \mathbb{R}[x]_r$ .
$\mathcal{M}(\mathbf{g})$	Quadratic module generated by the set $\mathbf{g}$ .
$\mathcal{M}(\mathbf{g})_r$	Quadratic module generated by the set $\mathbf{g}$ , truncated at degree $r$ .
$\mathcal{M}(\mathbf{x})$	Quadratic module generated by the set $\{x_1, \dots, x_n\}$ .
$\mathcal{T}(\mathbf{g})$	Preordering generated by the set $\mathbf{g}$ .
$\mathcal{T}(\mathbf{g})_r$	Preordering generated by the set $\mathbf{g}$ , truncated at degree $r$ .
$I(\mathbf{h})$	Ideal generated by the polynomial set $\mathbf{h}$ .
$I(\mathbf{h})_r$	Ideal generated by the polynomial set $\mathbf{h}$ , truncated at degree $r$ .
$I_{\Delta_n}$	Ideal generated by $\sum_{i=1}^n x_i - 1$ .
$I_{\mathbb{S}^{n-1}}$	Ideal generated by $\sum_{i=1}^n x_i^2 - 1$ .
$I_{G,r}$	Ideal generated by the graph $G$ , truncated at level $r$ .
$f^{(r)}$	Lasserre sum-of-squares hierarchy at order $r$ .

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A polynomial optimization problem asks for minimizing a polynomial function (cost) given a set of constraints (rules) represented by polynomial inequalities and equations. Many hard problems in combinatorial optimization and applications in operations research can be naturally encoded as polynomial optimization problems. A common approach for addressing such computationally hard problems is by considering variations of the original problem that give an approximate solution, and that can be solved efficiently. One such approach for attacking hard combinatorial problems and, more generally, polynomial optimization problems, is given by the so-called sum-of-squares approximations. This thesis focuses on studying whether these approximations find the optimal solution of the original problem.

We investigate this question in two main settings: 1) Copositive programs and 2) parameters dealing with independent sets in graphs. Among our main new results, we characterize the matrix sizes for which sum-of-squares approximations are able to capture all copositive matrices. In addition, we show finite convergence of the sums-of-squares approximations for maximum independent sets in graphs based on their continuous copositive reformulations.

We also study sum-of-squares approximations for parameters asking for maximum balanced independent sets in bipartite graphs. In particular, we find connections with the Lovász theta number and we design eigenvalue bounds for several related parameters when the graphs satisfy some symmetry properties.

LUIS FELIPE VARGAS BELTRÁN (Barrancabermeja, Colombia, 1995) Received his bachelor's and master's degrees in Mathematics from Universidad de Los Andes (2016 & 2019). In 2019 he joined the Networks and Optimization group at Centrum Wiskunde & Informatica (CWI) as a PhD candidate as a part of the Marie Skłodowska-Curie Innovative Training Network POEMA.

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