Exploiting symmetry in copositive programs via semidefinite hierarchies

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Abstract

Copositive programming is a relative young field which has evolved into a highly active research area in mathematical optimization. An important line of research is to use semidefinite programming to approximate conic programming over the copositive cone. Two major drawbacks of this approach are the rapid growth in size of the resulting semidefinite programs, and the lack of information about the quality of the semidefinite programming approximations. These drawbacks are an inevitable consequence of the intractability of the generic problems that such approaches attempt to solve.

To address such drawbacks, we develop customized solution approaches for highly symmetric copositive programs, which arise naturally in several contexts. For instance, symmetry properties of combinatorial problems are typically inherited when they are addressed via copositive programming. As a result we are able to compute new bounds for crossing number instances in complete bipartite graphs.

1 Introduction

Copositive programming (CP) has evolved into a highly active research field in the last fifteen years. The list of optimization problems to have CP representations has rapidly grown and includes *relaxations* for general quadratic programming [58], the standard quadratic programming problem [8, 12], the stable set problem [36], the quadratic assignment problem [55], graph partitioning problems [56], the chromatic number of a graph [26, 22], mixed integer linear programs under uncertainty [47], and the very general class of quadratic problems with linear and binary constraints [16].

The copositive formulation results of Burer [16] for QPs with linear as well as binary constraints, have been further extended in [2, 6, 10, 17]. More recently, a general class of polynomial optimization problems has been shown to be representable as linear optimization problems over the cone of *copositive tensors* [50].

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There is a large variety of algorithmic schemes to solve CPs. See for details [11, 14, 15, 18, 21, 35], or for an overview the surveys [7, 13, 23]. None of these approaches is polynomial time-efficient, which is not a surprise, as solving CPs is an NP-hard problem.

An important line of research is to use semidefinite programming (SDP) approximations to solve CPs (see Section 2.1). This line of research was started in [49], where a hierarchy of semidefinite programs is constructed to approximate CP. A hierarchy of linear programs to approximate the solution of CPs was introduced in [36], and a different hierarchy of semidefinite programs was introduced in [51]. The corresponding conic dual approximation schemes have been studied in [20]. However, the rapid growth in size and the lack of information about the quality are major drawbacks of these semidefinite programming approximations. These drawbacks are unavoidable, due to the intractability of the generic problems that these approaches attempt to solve.

Since the pioneering work of Gaterman and Parrilo [24] and Schrijver [59, 60], several authors have tackled the idea of exploiting the structure present in symmetric SDP problems. Firstly, using that the natural decision variables of a symmetric optimization problem are the orbits, not the points themselves, convex optimization problems can be restricted, via averaging, to the invariant feasible points (see e.g., Proposition 2). Secondly, symmetry reduction techniques for SDP (see [3], [19], and references therein) are based on the existence of an orthogonal transformation block diagonalizing the matrices invariant under the action of a given group. Generally, this block diagonalization contains several repeated blocks. Thus, this orthogonal transformation allows to represent an SDP constraint as a **number** of smaller SDP constraints, one for each (repeated) block.

Recent applications of SDP programs with symmetries are surveyed in [24, 30, 67] and include bounds on kissing numbers [4], bounds on crossing numbers [31, 33, 37], bounds on code sizes [25, 42, 60], truss topology design [5, 28], bounds on quadratic assignment problem [40], bounds on k-partitioning problem [34] and bounds on traveling salesman problem [32, 38].

Symmetry arise naturally in CPs, for instance, symmetry properties of combinatorial problems are typically preserved when they are addressed via CP. Since identifying and exploiting symmetries for the semidefinite constraint has proven to be successful, some authors suggested different techniques to tackle the symmetry on the lowest levels of the SDP -hierarchies used to approximate CPs. The applications include relaxations for the (fractional) chromatic number [27], and for the quadratic assignment problem and standard quadratic optimization problem with transitive automorphism groups [39].

In a related work, [57] exploits the special structure of Laserre's hierarchy [41] used to approximate polynomial programs. For this particular hierarchy their method improves upon the established methods. In a first step besides restricting to the invariant space, they also obtain a reduction on the size of the SDP (moment) matrices. In a second step they perform a block diagonalization to further reduce the size of SDP-constraints. A main difference between [57] and our work, is that the analytical reduction we provide in the first step depends only on computing orbits, while in their reduction they need to find a base of polynomial invariants.

1.1 Our Contribution

We develop new customized solution approaches for highly symmetric CPs. Our method falls into the systematic study of symmetry reduction initiated by Gatermann and Parillo [24], but falls out of the framework of equivalent representations of matrix *-algebras initiated by Schrijver [59, 60]. This new technique will allow to reduce in size every level in the SDP-hierarchy for CPs for any group acting on the underlying data including the case of nontransitive actions.

The novelty of our method lies in exploiting the structure of any level in the SDP-hierarchies used in CP for any group acting on the underlying data (including the case of nontransitive actions) to identify (Theorem 1) and analytically eliminate (Theorem 2) repeated blocks, **before** applying block diagonalization techniques (see Table 1.1). Each level of these hierarchies is a slice of a product of SDP-cones. We show how these slices can be represented using just one factor per orbit of certain action of the given group (see Theorem 1). Hence, the number of SDP-matrices and the size of the linear constraints defining each level of the hierarchy are greatly reduced (see, e.g., columns *Size description* in Table 2 versus Table 3). We call this outer symmetry reduction. In the reduced representation, a stabilizer from the original group acts independently *inside* each factor (i.e. each factor is fixed set-wise by the group). We call this inner symmetry. Existing methods to exploit symmetry for SDP, discussed in the introduction, can be applied to exploit the inner symmetry and further reduce the size of the SDP constraints via block diagonalization. However, depending on the inner symmetry structure, it could be advantageous not to apply this reduction when solving the optimization problem (see Section 4.1.1). Also, numerical issues could appear as the block diagonalized representation may contain irrational data. This is an important issue specially when the SDP problem is ill-possed (see [44] and [62]).

The algebraic simplicity of the outer symmetry reduction allows its application without sacrificing numerical tractability. To apply the outer symmetry reduction, it is enough to identify orbits (see Theorem 2). The well established methods for exploiting algebraic symmetry in SDP rely (next to identifying the orbits) on computing an equivalent representation of certain matrix algebras. Algorithms to perform such SDP symmetry reduction must deal with both orbit identification and more computationally involved procedures to perform equivalent algebraic representations (i.e. numerical block diagonalization).

Our methodology allows us to compute new bounds for crossing number instances (see Section 4.1.1), a problem which proved to be intractable to the existing well established methods.

We present the main structure of established methods and our methods in Table 1.1.

2 Preliminaries

2.1 Approximation hierarchies for Copositive Programming

Let $\mathbb{S}^n$ be the set of $n \times n$ symmetric matrices. We denote the cone of positive semidefinite matrices by:

$$\mathbb{S}^n_+ := \{A \in \mathbb{S}^n : x^\top A x \geq 0 \text{ for all } x \in \mathbb{R}\}$$

and the set of copositive matrices by:

$$\mathcal{C}^n := \{A \in \mathbb{S}^n : x^\top A x \geq 0 \text{ for all } x \geq 0\}.$$

We will drop the superscript n, and use $\mathbb{S}$, $\mathbb{S}_+$, $\mathcal{C}$, when clear from context.

Approximations hierarchies for $\mathcal{C}$ are based on conditions which ensure non-negativity of polynomials. For a given symmetric matrix $M \in \mathbb{S}$, consider its associated quadratic form

$$q_M(x) := x^\top M x.$$

Let $x^{\circ 2} = x \circ x$ be the elementwise square of x. Then, $M \in \mathcal{C}$ if and only if $q_M(x^{\circ 2}) \geq 0$ for all $x \in \mathbb{R}^n$. Parrilo [49] defined the following hierarchy of cones

$$\mathcal{K}^r := \left\{ M \in \mathbb{S} : \left(\sum_{i=1}^n x_i^2 \right)^r q_M(x^{\circ 2}) \text{ has an sos decomposition} \right\}.$$

Established methods			
	What	How	Effect
S1	Restriction to invariant subspace	Find basis using orbits	Reduction in the number of variables
Step 2	Block diagonalization and Elimination of repeated blocks	Represent invariant matrices under the action of the **given group** as direct sum of irreducible representations	Reduction of the **size** of SDP constraint(s) and Reduction of the **number** of SDP constraint(s)

Our method			
	What	How	Effect
OUTER	Restriction to invariant subspace and Elimination of repeated blocks	Find basis using orbits **and apply Theorem 2**	Reduction in the number of variables and Reduction of the **number** of SDP constraint(s)
INNER	Block diagonalization	Represent invariant matrices under the action of the **stabilizer group** as direct sum of irreducible representations	Reduction of the **size** of SDP constraint(s)

Table 1: Symmetry reduction techniques

Parrilo showed the cones $\mathcal{K}^r$ approximate $\mathcal{C}$ in the sense that $\mathbb{S}_+ + \mathcal{N} = \mathcal{K}^0 \subseteq \mathcal{K}^1 \subseteq \cdots \subseteq \mathcal{C}$, and $\text{int}(\mathcal{C}) \subseteq \bigcup_{r\in\mathbb{N}} \mathcal{K}^r$. Since the sos condition can be written as a system of linear matrix inequalities (LMI), optimizing over $\mathcal{K}^r$ can be formulated as a semidefinite program.

Using that $M \in \mathcal{C}$ if and only if $q_M(x)$ is non-negative on the standard simplex, de Klerk and Pasechnik [36] obtain the following hierarchy of polyhedral cones approximating $\mathcal{C}$:

$$\mathcal{C}^r := \left\{ M \in \mathbb{S} \colon \left(e^\top x\right)^r x^\top M x \text{ has only nonnegative coefficients} \right\}.$$

From Polya theorem [54] every strictly copositive matrix lies in some cone $\mathcal{C}^r$ for r sufficiently large.

Peña, Vera and Zuluaga [51] derive another SDP hierarchy of cones approximating $\mathcal{C}$. Adopting standard multiindex notation, where for a given multiindex $\beta \in \mathbb{N}^n$ we have $|\beta| := \beta_1 + ... + \beta_n$

and $x^\beta := x_1^{\beta_1}\cdots x_n^{\beta_n}$ they define the cones

$$\mathcal{Q}^r := \left\{ M \in \mathbb{S} \colon \left(e^\top x\right)^r x^\top M x = \sum_{\beta\in\mathbb{N}^n, |\beta|=r} x^\beta x^\top (P_\beta + N_\beta)x,\ P_\beta \in \mathbb{S}_+, N_\beta \in \mathcal{N} \right\}.$$

They show that $\mathcal{C}^r \subseteq \mathcal{Q}^r \subseteq \mathcal{K}^r$ for all $r \in \mathbb{N}$, with $\mathcal{Q}^r = \mathcal{K}^r$ for $r = 0, 1$. Similar to the case of $\mathcal{K}^r$, the condition $M \in \mathcal{Q}^r$ can be written as a system of LMIs. Optimizing over $\mathcal{Q}^r$ is therefore again an SDP.

Our new technique can be applied to any of the three previously defined family of cones. For notational convenience, we present these hierarchies in an unified manner. Let

$$\mathbb{H}_k^r := \left\{ M \in \mathbb{S} \colon \left(e^\top x\right)^r x^\top M x = \sum_{j=r+2-k}^{r+2} \sum_{\beta\in\mathbb{N}_j^n} x^\beta \sigma_\beta(x),\ \sigma_\beta(x) \in \Sigma_{r+2-|\beta|} \right\}, \tag{1}$$

where Σ_d denotes the sos polynomials of degree d for any d, and $\mathbb{N}_d^n := \{\beta \in \mathbb{N}^n \colon |\beta| = d\}$ for any d and n.

In the case $k = 0$, using that a degree 0 polynomial is an SOS if and only if it is a non-negative constant we obtain $\mathcal{C}^r = \mathbb{H}_0^r$. In the case $k = 2$ using

$$\left\{ \sum_{\beta\in\mathbb{N}_r^n} x^\beta x^\top N_\beta x : N_\beta \in \mathbb{R}_+^{n\times n} \right\} = \left\{ \sum_{\beta\in\mathbb{N}_{r+2}^n} c_\beta x^\beta : c_\beta \geq 0 \right\}$$

we obtain $\mathcal{Q}^r = \mathbb{H}_2^r$. Finally, it was shown in [52, Prop. 9] that for a homogenous polynomial $p(x)$ of degree d, $p(x^{\circ 2})$ is an sos if and only if

$$p(x) = \sum_{j=0}^{d} \sum_{\beta\in\mathbb{N}_j^n} x^\beta \sigma_\beta(x) \text{ with } \sigma_\beta(x) \in \Sigma_{d-|\beta|}$$

which implies $\mathcal{K}^r = \mathbb{H}_k^r$, for any $k \geq r + 2$.

2.2 Symmetry in Conic Programming

We encode the symmetry of the problem trough group actions. Let $\mathcal{P}_n$ be the group of $n \times n$ permutation matrices under matrix multiplication. We restrict our attention to subgroups of $\mathcal{P}_n$ because every group action over a finite set is in correspondence in a canonical way to a group action where the acting group G is a subgroup of $\mathcal{P}_n$ for an appropriate n.

We will consider the natural action of G on $\mathbb{R}^n$ (respectively $\mathbb{R}[x]$ and $\mathbb{S}$) defined by $x^P := Px$ (respectively $q(x)^P := q(Px)$ and $M^P := P^\top M P$) for any $P \in G$. These actions are consistent in the sense that for any $x \in \mathbb{R}^n$, $p(x) \in \mathbb{R}[x]$ and $M \in \mathbb{S}$, we have $p(x)^P = p(x^P)$ and $q_M(x)^P = x^\top P^\top M P x = q_{M^P}(x)$ for all $P \in G$.

For any set U on which G acts, $\mathrm{Orb}_G(U)$ is the set of orbits of U under the action of G, $U^G = \{u \in U \colon u^P = u \text{ for all } P \in G\}$ is the set of *G-invariant* elements of U. The mapping $u \mapsto R_G(u) := \frac{1}{|G|}\sum_{P\in G} u^P$, is called the *group average* or *Reynolds operator*. Notice that for any $u \in U$ we have that $R_G(u)$ is G-invariant, moreover u is G-invariant if and only if $R_G(u) = u$.

Lemma 1. *Let U be a vector space of dimension d. Let G be a group acting on U. Then* *(i)* U^G *is a subspace of* U*.*

(ii) Let $B = \{b_1, \ldots, b_d\}$ *be a base for* U*. If* B *is closed under the action of* G*, then* $\{R_G(b_1), \ldots, R_G(b_d)\}$ *is a base for* U^G*. Moreover* $\dim(U^G) = |\operatorname{Orb}_G(B)|$*.*

We consider the primal-dual conic programming problem in matrix variable:

$$\begin{array}{llcll} \min & \operatorname{tr}(CX) & \qquad & \max & b^\top y \\ \text{s.t.} & \operatorname{tr}(A_i X) = b_i,\ i = 1, ..., m & & \text{s.t.} & \sum_{i=1}^m y_i A_i + S = C \\ & X \in \mathcal{K} & & & y \in \mathbb{R}^m,\ S \in \mathcal{K}^* \end{array} \tag{2}$$

where $C, A_1, \ldots, A_m \in \mathbb{S}$, $b \in \mathbb{R}^m$, $\mathcal{K} \subseteq \mathbb{S}$ is a convex cone, and $\mathcal{K}^* := \{S \in \mathbb{S} : \operatorname{tr}(SX) \geq 0\ \forall X \in \mathcal{K}\}$ is the dual cone of $\mathcal{K}$.

Definition 1 (Conic Programming Symmetry)**.** *Let* $G \subseteq \mathcal{P}_n$ *be a group of permutation matrices. We say that the primal-dual pair* (2) *is* G*-invariant if the following holds for the natural action of* G *on* $\mathbb{S}$*:*

(S1) the matrix C *is point-wise invariant: For all* $P \in G$*,* $P^\top C P = C$

(S2) $\{(A_i, b_i) : i = 1, ..., m\}$ *is set-wise invariant: For all* $P \in G$*,* $\{(P^\top A_i P, b_i) : i = 1, ..., m\} = \{(A_i, b_i) : i = 1, ..., m\}$

(S3) $\mathcal{K}$ *is closed under the action of* G*: For all* $M \in \mathcal{K}$ *and all* $P \in G$*,* $P^\top M P \in \mathcal{K}$*.*

Remark 2. *For the case of semidefinite invariant programs (i.e. the case* $\mathcal{K} = \mathbb{S}_+$*), Definition 1 is slightly more general than the standard definition (see e.g. [30]) where (S2) is replaced by the more restrictive*

(S2) For* $i = 1, ..., m$*,* A_i *is point-wise invariant: For all* $P \in G$*,* $P^\top A_i P = A_i$*,*

and (S3) holds due to the properties of the semidefinite cone.

Condition (S2) is equivalent to the fact that each $P \in G$ permutes the order of the linear constrains in (2). Let $Q_P \in \mathcal{P}_m$ be the corresponding permutation matrix, namely Q_P is defined by $Q_{P,ij} = 1$ if and only if $P^\top A_i P = A_j$. We define $\tilde{G} = \{Q_P : P \in G\} \subseteq \mathcal{P}_m$. Notice that (S2) implies b is $\tilde{G}$-invariant.

The following proposition extends to the more general framework of conic programming a well known result in the context of SDP, that one can restrict the optimization of the primal-dual pair (2) to $\mathcal{K}^G$. When $\mathcal{K} = \mathbb{S}_+$ this was shown previously by Gatermann and Parrilo in [24], de Klerk in [30], among others.

Proposition 2. *Assume the primal-dual pair* (2) *is* G*-invariant. Then the primal-dual pair* (2) *is equivalent to the pair*

$$\begin{array}{llcll} \min & \operatorname{tr}(CX) & \qquad & \max & b^\top y \\ \text{s.t.} & \operatorname{tr}(R_G(A_i) X) = b_i,\ i = 1, ..., m & & \text{s.t.} & \sum_{i=1}^m y_i R_G(A_i) + S = C \\ & X \in \mathcal{K}^G & & & y \in (\mathbf{R}^m)^{\tilde{G}},\ S \in (\mathcal{K}^*)^G \end{array} \tag{3}$$

Proof. If $X \in \mathbb{S}^G$ we have $\mathrm{tr}\,(A_iX) = \mathrm{tr}\,(A_iR_G(X)) = \mathrm{tr}\,(R_G(A_i)X) = b_i$. Also, if $y \in (\mathbf{R}^m)^{\tilde{G}}$ then $\sum_{i=1}^m y_iA_i$ is G-invariant. Thus if the tuple (X, y, S) is feasible for the pair (3) then it is feasible for the pair (2) and has the same objective values in both pairs (3) and (2) . Conversely if the tuple (X, y, S) is feasible for the pair (2), following the lines of the proof of [24, Theorem 3.3], defining $\tilde{R}_G(y) = \frac{1}{|G|}\sum_{P\in G} Q_Py$, the tuple $(R_G(X), \tilde{R}_G(y), R_G(S))$ is feasible for the pair (3) and, $\mathrm{tr}\,(CX) = \mathrm{tr}\,(CR_G(X))$ and $b^\top y = b^\top \tilde{R}_G(y)$. □ □

Proposition 2 implicitly reduces the size of the problem pair (2). On one hand, $\mathbb{S}^G$ is a subspace of $\mathbb{S}$, and thus, the pair (3) requires less variables than the pair (2). On the other hand, the number of linear equations in (3) reduces from m to the number of orbits (say m_1) of the action of $\tilde{G}$ on $\{1, \dots, m\}$, as $R_G(A_i) = R_G(A_j)$ when i and j are in the same orbit.

The pair (3) is not a primal dual pair as in general $(\mathcal{K}^G)^* \supset \mathcal{K}^*$. However they are primal-dual in the restricted subspace $\mathbb{S}^G$. In Proposition 3 we prove this claim, and present an explicit form of the symmetry reduction implicitly given in Proposition 2.

From Lemma 1, $\mathbb{S}^G$ is a subspace of $\mathbb{S}$. Fix $\{B_1, ..., B_d\}$, where $d = \dim(\mathbb{S}^G)$, an orthonormal basis with respect to the usual trace inner product of $\mathbb{S}^G$. Similarly fix $\{e_j : j = 1, \dots, m_1\}$ an orthonormal basis, with respect to the 1-norm, for $(\mathbb{R}^m)^{\tilde{G}}$. We can write the variable and data matrices of the pair (3) as follows:

$$\begin{gathered} X = \textstyle\sum_{j=1}^d x_jB_j, \quad y = \sum_{j=1}^{m_1} u_je_j, \quad S = \sum_{j=1}^d s_jB_j \\ R_G(A_i) = \textstyle\sum_{j=1}^d \alpha_{ij}B_j \;\forall i = 1, ..., m_1, \quad b = \sum_{j=1}^{m_1} \beta_je_j, \quad C = \sum_{j=1}^d \gamma_jB_j, \end{gathered} \tag{4}$$

with $x, \gamma, s \in \mathbb{R}^d$, $u, \beta \in R^{m_1}$ and $\alpha \in \mathbb{R}^{d\times m_1}$.

Proposition 3. *Assume the primal-dual pair* (2) *is G-invariant. Then the pair* (2) *is equivalent to the following primal-dual pair*

$$\begin{array}{lllll} \min & \gamma^\top x & \qquad & \max & \beta^T u \\ \text{s.t.} & \alpha^\top x = \beta, & & \text{s.t.} & \alpha u + s = \gamma \\ & \sum_{j=1}^d x_jB_j \in \mathcal{K}^G. & & & u \in \mathbb{R}^{m_1}, \quad \sum_{j=1}^d s_jB_j \in (\mathcal{K}^*)^G. \end{array} \tag{5}$$

Proof. Using the linearity of the trace operator, the orthogonality of the basis $\{B_1, ..., B_d\}$, and (4) we obtain that (3) is equivalent to (5).

Now we prove that the pair (5) is a primal-dual pair. To this end, let

$$A := \{x \in \mathbb{R}^d : \sum_{j=1}^d x_jB_j \in \mathcal{K}^G\} \text{ and } D := \{s \in \mathbb{R}^d : \sum_{j=1}^d s_jB_j \in (\mathcal{K}^*)^G\}.$$

We need to show $D = A^*$. Let $s \in D$, for any $x \in A$ we have that $x^\top s = \mathrm{tr}\left(\left(\sum_{i=1}^d x_iB_i\right)\left(\sum_{i=1}^d s_iB_i\right)\right) \geq 0$ and then $s \in A^*$. Conversely, let $s \in A^*$. We have $\mathrm{tr}\left(\left(\sum_{i=1}^d x_iB_i\right)\left(\sum_{i=1}^d s_iB_i\right)\right) = x^\top s \geq 0$ for all $x \in A$. Hence $S = \sum_{i=1}^d s_iB_i \in (\mathcal{K}^G)^*$. Now, for any $X \in \mathcal{K}$, we have $\mathrm{tr}\,(XS) = \mathrm{tr}\,(XR_G(S)) = \mathrm{tr}\,(R_G(X)S) \geq 0$, which implies $S \in \mathcal{K}^*$. Thus $s \in D$. □ □

To use the size reduction given by the pair (5), it is necessary to express the conditions $\sum_{j=1}^d x_jB_j \in \mathcal{K}^G$ and/or $\sum_{j=1}^d s_jB_j \in (\mathcal{K}^*)^G$ in a *reduced* way. That is to reduce the matrix size of the conic restriction. We present this reduced form for the cones $(\mathcal{C}^r)^G$, $(\mathcal{Q}^r)^G$ and $(\mathcal{K}^r)^G$ for any $G \subseteq \mathcal{P}_n$ in Section 3.

3 Exploiting symmetry to represent $(\mathbb{H}_k^r)^G$

Fix $G \subseteq \mathcal{P}_n$ a group of permutation matrices. We construct an explicit reduced representation of $(\mathbb{H}_k^r)^G$ for any r and k, providing symmetry reductions for the cones $(\mathcal{C}^r)^G$, $(\mathcal{Q}^r)^G$ and $(\mathcal{K}^r)^G$. To this end we will make use of the following notation.

Let $\mathbb{N}^{\{2\}}$ be the set of unordered pairs $\{\{i,j\} : 1 \leq i \leq j \leq n\}$ Consider the following basis for $\mathbb{S}$: $B_{\mathbb{S}} = \{E^{ij} : \{i,j\} \in \mathbb{N}^{\{2\}}\}$, where E^{ij} is the matrix with zeros everywhere except for a $\frac{1}{|\{i,j\}|}$ in positions (i,j) and (j,i) . Applying part (ii) of Lemma 1 we obtain that the space $\mathbb{S}^G$ has the basis $B_{\mathbb{S}^G} = \{E^{\mathcal{J}} : \mathcal{J} \in \mathrm{Orb}_G(\mathbb{N}^{\{2\}})\}$, where for each $\mathcal{J} \in \mathrm{Orb}_G(\mathbb{N}^{\{2\}})$ the matrix $E^{\mathcal{J}} = R_G(E^{ij})$ for any $\{i,j\} \in \mathcal{J}$.

Let $\mathbf{H}_d[x]$ be the space of homogeneous degree d polynomials. Notice that $\mathbf{H}_d[x]$ is closed under the action of G. Consider the standard monomial base for $\mathbf{H}_d[x]$, $B^d_{mon} = \{x^\beta : \beta \in \mathbb{N}^n_d\}$. Applying part (ii) of Lemma 1 we obtain that the space $\mathbf{H}_d[x]^G$ has as basis $B^d_{G-mon} = \{p_{\mathcal{I}}(x) : \mathcal{I} \in \mathrm{Orb}_G(\mathbb{N}^n_d)\}$, where for each $\mathcal{I} \in \mathrm{Orb}_G(\mathbb{N}^n_d)$, the polynomial $p_{\mathcal{I}}(x) = R_G(x^\beta)$ for any $\beta \in \mathcal{I}$.

Our election of basis is consistent with the natural isomorphism between $\mathbb{S}$ and $\mathbf{H}_2[x]$, as this isomorphism send basis elements to basis elements. In particular, we identify the sets $\mathbb{N}^{\{2\}}$ and $\mathbb{N}^n_2$, as well as their corresponding orbits.

Theorem 1. *Let $G \subseteq \mathcal{P}_n$ be a group of permutation matrices. Let $r, k \geq 0$. Then for any $M \in \mathbb{S}$, $M \in (\mathbb{H}_k^r)^G$ if and only if for each $j = r+2-k, \ldots, r+2$ and each $\beta \in \mathbb{N}^n_j$ there exist $\sigma_\beta(x) \in \Sigma_{r+2-j}$ such that*

(i) $\left(e^\top x\right)^r x^\top M x = \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} x^\beta \sigma_\beta(x)$

(ii) For each $j = r+2-k, \ldots, r+2$, each $\beta \in \mathbb{N}^n_j$ and each $P \in G$, $\sigma_{P\beta}(x) = \sigma_\beta(P^\top x)$.

Proof. Assume $M \in (\mathbb{H}_k^r)^G$. Then by definition of $\mathbb{H}_k^r$ there are $\sigma_\beta(x) \in \Sigma_{r+2-|\beta|}$ with $\beta \in \mathbb{N}^n_{[r+2-k,r+2]}$ such that (i) holds. As M is G-invariant, $M = \frac{1}{|G|}\sum_{P \in G} P^\top M P$, therefore

$$
\begin{aligned}
\left(e^\top x\right)^r x^\top M x &= \left(e^\top x\right)^r \frac{1}{|G|} \sum_{P \in G} x^\top P^\top M P x \\
&= \frac{1}{|G|} \sum_{P \in G} \left(e^\top (Px)\right)^r (Px)^\top M (Px) && (\text{using } e^\top P = e^\top) \\
&= \frac{1}{|G|} \sum_{P \in G} \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} (Px)^\beta \sigma_\beta(Px) && (\text{using (i)}) \\
&= \frac{1}{|G|} \sum_{P \in G} \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} x^{P^\top \beta} \sigma_\beta(Px) \\
&= \frac{1}{|G|} \sum_{P \in G} \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} x^{\beta} \sigma_{P\beta}(Px) && (\text{subs. } \beta \to P\beta) \\
&= \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} x^{\beta} \frac{1}{|G|} \sum_{P \in G} \sigma_{P\beta}(Px) \\
&= \sum_{j=r+2-k}^{r+2} \sum_{\beta \in \mathbb{N}^n_j} x^{\beta} \hat{\sigma}_\beta(x)
\end{aligned}
$$

where $\hat{\sigma}_\beta(x) := \frac{1}{|G|}\sum_{P\in G}\sigma_{P\beta}(Px)$. For each $j = r+2-k,\ldots,r+2$ and each $\beta\in\mathbb{N}^n_j$, $\hat{\sigma}_\beta(x)\in\Sigma_{r+2-j}$. Also, for any $Q\in G$, we have

$$\begin{aligned}\hat{\sigma}_\beta(Qx) &= \frac{1}{|G|}\sum_{P\in G}\sigma_{P\beta}(PQx)\\ &= \frac{1}{|G|}\sum_{P\in G}\sigma_{PQ^\top\beta}(Px) && \text{(subs. } P\to PQ^\top)\\ &= \hat{\sigma}_{Q^\top\beta}(x).\end{aligned}$$

Thus $\hat{\sigma}_\beta(x)$ with $\beta\in\mathbb{N}^n_j$, $j=r+2-k,\ldots,r+2$ satisfy (i) and (ii).

Now let $\sigma_\beta(x)\in\Sigma_{r+2-|\beta|}$ with $\beta\in\mathbb{N}^n_j$, $j=r+2-k,\ldots,r+2$ be such that (i) and (ii) hold. Then (i) implies $M\in\mathbb{H}^r_k$. To show $M\in(\mathcal{H}^r_k)^G$ consider $P\in G$. We have

$$\begin{aligned}\big(e^\top x\big)^r x^\top P^\top MPx &= \big(e^\top(Px)\big)^r(Px)^\top M(Px) && \text{(from } e^\top P = e^\top)\\ &= \sum_{j=k}^{r+2}\sum_{\beta\in\mathbb{N}^n_j}(Px)^\beta\sigma_\beta(Px) && \text{(using (i))}\\ &= \sum_{j=k}^{r+2}\sum_{\beta\in\mathbb{N}^n_j}x^{P^\top\beta}\sigma_{P^\top\beta}(x) && \text{(from (ii))}\\ &= \sum_{j=k}^{r+2}\sum_{\beta\in\mathbb{N}^n_j}x^\beta\sigma_\beta(x) && \text{(subs. } \beta\to P\beta)\\ &= \big(e^\top x\big)^r x^\top Mx && \text{(from (i))}\end{aligned}$$

which implies $P^\top MP = M$. □ □

When written in terms of the SDP representation of SOS Theorem 1 takes the form

$$\{y\in\mathbb{S}^n : Ly = Ts,\ s\in\prod_{\beta\in I}\mathbb{S}^{n_\beta}_+\}^G = \{y\in\mathbb{S}^n : Ly = \tilde{T}z,\ z\in\prod_{\beta\in J}(\mathbb{S}^{n_\beta}_+)^{G_j}\},$$

for some J and I with $J\subset I$ and $|J| << |I|$. Notice that in the proof of Theorem 1 not only the product structure of the cone is important but also the particular structure of the linear transformations L and T in the definition of the cone $\mathbb{H}^r_k$.

Given $\beta\in\mathbb{N}^n_d$, we denote by $G\beta := \{P\beta : P\in G\}$ the orbit of β under the action of G and by $\mathrm{Orb}_G(\mathbb{N}^n_d) = \{G\beta : \beta\in\mathbb{N}^n_d\}$ the set of all orbits of this action. Further, let $\mathrm{Fix}_G(\beta) = \{P\in G : P\beta = \beta\}$ the stabilizer of β in G.

Fix $r+2-k\le j\le r+2$, fix $\mathcal{O}\in\mathrm{Orb}_G(\mathbb{N}^n_d)$ and fix $\beta_\mathcal{O}\in\mathcal{O}$ a representative for the orbit. Using condition (ii) in Theorem 1 we obtain the following size-reduction for the SOS representation of $(\mathbb{H}^r_k)^G$.

- *Outer symmetry reduction*: Only one SOS is needed for the whole orbit $\mathcal{O}$ in the representation, as one can define $\sigma_\beta(x) = \sigma_{\beta_\mathcal{O}}(P^\top x)$ if $\beta = P\beta_0$.

- *Inner symmetry reduction*: $\sigma_{\beta_\mathcal{O}}(x)$ can be taken $\mathrm{Fix}_G(\beta_\mathcal{O})$-invariant.

The outer symmetry reduction is a reduction in the number of PSD matrix variables needed to represent $(\mathbb{H}_k^r)^G$. Let $N_d = \binom{n+d-1}{d}$ the number of degree d monomials in n variables. For each $0 \leq d \leq k$, definition (1) of $\mathbb{H}_k^r$ requires N_{r+2-d} SOS of degree d, that is, N_{r+2-d} SDP matrices of size N_d. Using the outer symmetry reduction from Theorem 1 only $|\operatorname{Orb}_G(\mathbb{N}^n_{r+2-d})|$ SOS of degree d are required. The reduction on the number of SDP variables depends on the number of orbits of the action of the group. For example if the group is transitive, the reduction is at least a factor of n for any r, in particular, only one SOS is required when $r = 1$.

The inner symmetry of the PSD-matrix variables obtained after using the outer symmetry could be exploited to reduce the size of the corresponding SDP-constraint using the well established techniques mentioned in the introduction. However, depending of the structure of the inner symmetry it might not be advantageous to exploit such symmetry. For instance, this will be the case if the stabilizer group $\operatorname{Fix}_G(\beta_{\mathcal{O}})$ or the SDP-variable representing $\sigma_{\beta_{\mathcal{O}}}(x)$ are too small. More importantly, for SDP programs with large data, techniques to obtain block-diagonalization by exploiting symmetry come along with a numerical issue. The algebra which contains the SDP data is a coherent algebra. Hence it has basis $\mathcal{B}_{orig}$ of highly sparse {0,1}-matrices, easy to store in the computer memory. The basis $\mathcal{B}_{equiv}$ of an equivalent representation of this algebra, is obtained applying a suitable unitary transformation to every element in $\mathcal{B}_{orig}$. These new basis, $\mathcal{B}_{equiv}$, has a fully dense block-structure with real / complex values. The precision storage of these values has an influence on the precision of the computed optimal value for the optimization problem. As a consequence storing and using the basis $\mathcal{B}_{equiv}$ might render numerical intractability. For a detailed example see Section 4.1.1

The number of linear constrains used in the representation of $\mathbb{H}_k^n$ is also reduced when using Theorem 1. In (1) there are N_{r+2} such constrains, as we need to express the equality of two polynomials of degree $r+2$. After applying Theorem 1 the two polynomials are still of degree $r+2$, but they are G-invariant. Therefore, using a G-invariant basis the number of linear equations in this system reduces to $|\operatorname{Orb}_G(\mathbb{N}^n_{r+2})|$.

The symmetry-reductions obtained from Theorem 1 are made explicit in Theorem 2. To state the theorem, for each $j = 0, \ldots, k$ and each $\mathcal{O} \in \operatorname{Orb}_G(\mathbb{N}^n_{r+2-j})$ fix $\beta_{\mathcal{O}} \in \mathcal{O}$ and for each $\mathcal{I} \in \operatorname{Orb}_{\operatorname{Fix}_G(\beta_{\mathcal{O}})}(\mathbb{N}^n_j)$ fix $\alpha^{\mathcal{O}}_{\mathcal{I}} \in \mathcal{I}$.

Theorem 2. *Let $m_{\mathcal{J}} \in \mathbb{R}$ for $\mathcal{J} \in \operatorname{Orb}_G(\mathbb{N}^n_2)$ be given. Let $M = \sum_{\mathcal{J}\in\operatorname{Orb}_G(\mathbb{N}^n_2)} m_{\mathcal{J}} E^{\mathcal{J}}$. Then $M \in (\mathbb{H}_k^r)^G$ if and only if there exist $s^{\mathcal{O}}_{\mathcal{I}} \in \mathbb{R}$ with $\mathcal{I} \in \operatorname{Orb}_{\operatorname{Fix}_G(\beta_{\mathcal{O}})}(\mathbb{N}^n_j)$, $\mathcal{O} \in \operatorname{Orb}_G(\mathbb{N}^n_{r+2-j})$, $j = 0, \ldots, k$ such that the following holds*

(i) For each $\mathcal{U} \in \operatorname{Orb}_G(\mathbb{N}^n_{r+2})$

$$\sum_{\substack{\mathcal{J}\in\operatorname{Orb}_G(\mathbb{N}^n_2)\\ \mathcal{I}\in\operatorname{Orb}_{\operatorname{Fix}_G(\beta_{\mathcal{J}})}(\mathbb{N}^n_r):\\ \beta_{\mathcal{J}}+\alpha^{\mathcal{J}}_{\mathcal{I}}\in\mathcal{U}}} \binom{r}{\alpha^{\mathcal{J}}_{\mathcal{I}}} |\mathcal{I}| m_{\mathcal{J}} = \sum_{j=0}^{k} \sum_{\substack{\mathcal{O}\in\operatorname{Orb}_G(\mathbb{N}^n_{r+2-j})\\ \mathcal{I}\in\operatorname{Orb}_{\operatorname{Fix}_G(\beta_{\mathcal{O}})}(\mathbb{N}^n_j):\\ \beta_{\mathcal{O}}+\alpha^{\mathcal{O}}_{\mathcal{I}}\in\mathcal{U}}} |\mathcal{O}| s^{\mathcal{O}}_{\mathcal{I}}$$

(ii) For each $j = 0, \ldots, k$ for each $\mathcal{O} \in \operatorname{Orb}_G(\mathbb{N}^n_{r+2-j})$,

$$\sum_{\mathcal{I}\in\operatorname{Orb}_{\operatorname{Fix}_G(\beta_{\mathcal{O}})}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_{\operatorname{Fix}_G(\beta_{\mathcal{O}})}(x^{\alpha^{\mathcal{O}}_{\mathcal{I}}}) \in \Sigma_j$$

Proof. Assume $M \in (\mathbb{H}_k^r)^G$. Let σ_β be given by Theorem 1. Fix $0 \leq j \leq k$, we have

$$\sum_{\beta\in\mathbb{N}^n_{r+2-j}} x^\beta \sigma_\beta(x) = \sum_{\mathcal{O}\in\operatorname{Orb}_G(\mathbb{N}^n_{r+2-j})} \sum_{\beta\in\mathcal{O}} x^\beta \sigma_\beta(x)$$

$$= \sum_{\mathcal{O}\in \mathrm{Orb}_G(\mathbb{N}^n_{r+2-j})} \frac{|\mathcal{O}|}{|G|} \sum_{P\in G} x^{P\beta_{\mathcal{O}}} \sigma_{P\beta_{\mathcal{O}}}(x)$$

$$= \sum_{\mathcal{O}\in \mathrm{Orb}_G(\mathbb{N}^n_{r+2-j})} \frac{|\mathcal{O}|}{|G|} \sum_{P\in G} (P^\top x)^{\beta_{\mathcal{O}}} \sigma_{\beta_{\mathcal{O}}}(P^\top x) \qquad \text{(using theorem 1(ii))}$$

$$= \sum_{\mathcal{O}\in \mathrm{Orb}_G(\mathbb{N}^n_{r+2-j})} |\mathcal{O}| R_G(x^{\beta_{\mathcal{O}}} \sigma_{\beta_{\mathcal{O}}}(x)). \tag{6}$$

Now, let $\mathcal{O} \in \mathrm{Orb}_G(\mathbb{N}^n_{r+2-j})$. Let $G_{\mathcal{O}} = \mathrm{Fix}_G(\beta_{\mathcal{O}})$. As $\sigma_{\beta_{\mathcal{O}}}(x) \in \mathbf{H}_j[x]^{G_{\mathcal{O}}}$, we can write $\sigma_{\beta_{\mathcal{O}}}(x) = \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_{G_{\mathcal{O}}}(x^{\alpha^{\mathcal{O}}_{\mathcal{I}}})$, where $s^{\mathcal{O}}_{\mathcal{I}} \in \mathbb{R}$ for each $\mathcal{I} \in \mathrm{Orb}_{G_{\mathcal{O}}}$, and (ii) follows. We also have,

$$R_G(x^{\beta_{\mathcal{O}}} \sigma_{\beta_{\mathcal{O}}}(x)) = R_G\left(x^{\beta_{\mathcal{O}}} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_{G_{\mathcal{O}}}(x^{\alpha^{\mathcal{O}}_{\mathcal{I}}}) \right)$$

$$= \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_G\Big(x^{\beta_{\mathcal{O}}} R_{G_{\mathcal{O}}}(x^{\alpha^{\mathcal{O}}_{\mathcal{I}}}) \Big)$$

$$= \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_G\Big(R_{G_{\mathcal{O}}}(x^{\beta_{\mathcal{O}}+\alpha^{\mathcal{O}}_{\mathcal{I}}}) \Big) \qquad (\text{ as } \beta_{\mathcal{O}} \in \mathbb{N}^{G_{\mathcal{O}}}_{r+2-j})$$

$$= \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} R_G(x^{\beta_{\mathcal{O}}+\alpha^{\mathcal{O}}_{\mathcal{I}}}) \tag{7}$$

Putting (6) and (7) together we obtain

$$\sum_{\beta\in\mathbb{N}^n_{r+2-j}} x^\beta \sigma_\beta(x) = \sum_{\mathcal{O}\in \mathrm{Orb}_G(\mathbb{N}^n_{r+2-j})} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{O}}}(\mathbb{N}^n_j)} s^{\mathcal{O}}_{\mathcal{I}} |\mathcal{O}| R_G(x^{\beta_{\mathcal{O}}+\alpha^{\mathcal{O}}_{\mathcal{I}}}). \tag{8}$$

Similarly,

$$\left(e^\top x\right)^r x^\top M x = \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^{\{2\}})} m_{\mathcal{J}} x^\top M^{\mathcal{J}} x \left(e^\top x\right)^r$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^n_2)} m_{\mathcal{J}} R_G(x^{\beta_{\mathcal{J}}}) \left(e^\top x\right)^r$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^n_2)} m_{\mathcal{J}} R_G\Big(x^{\beta_{\mathcal{J}}} \left(e^\top x\right)^r\Big)$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^n_2)} m_{\mathcal{J}} R_G\left(x^{\beta_{\mathcal{J}}} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{J}}}(\mathbb{N}^n_j)} \sum_{\alpha\in\mathcal{I}} \binom{r}{\alpha} x^\alpha \right)$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^n_2)} m_{\mathcal{J}} R_G\left(x^{\beta_{\mathcal{J}}} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{J}}}(\mathbb{N}^n_j)} \binom{r}{\alpha^{\mathcal{J}}_{\mathcal{I}}} |\mathcal{I}| R_{G_{\mathcal{J}}}\Big(x^{\alpha^{\mathcal{J}}_{\mathcal{I}}}\Big) \right)$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}^n_2)} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{J}}}(\mathbb{N}^n_j)} \binom{r}{\alpha^{\mathcal{J}}_{\mathcal{I}}} |\mathcal{I}| m_{\mathcal{J}} R_G\Big(x^{\beta_{\mathcal{J}}} R_{G_{\mathcal{J}}}\Big(x^{\alpha^{\mathcal{J}}_{\mathcal{I}}}\Big)\Big)$$

$$= \sum_{\mathcal{J}\in \mathrm{Orb}_G(\mathbb{N}_2^n)} \sum_{\mathcal{I}\in \mathrm{Orb}_{G_{\mathcal{J}}}(\mathbb{N}_j^n)} \binom{r}{\alpha_{\mathcal{I}}^{\mathcal{J}}} |\mathcal{I}| m_{\mathcal{J}} R_G\left(x^{\beta_{\mathcal{J}}+\alpha_{\mathcal{I}}^{\mathcal{J}}}\right) \tag{9}$$

From (8) and (9), (i) follows.

Now, assume the statement of the theorem holds. For each $j = 0, \ldots, k$, and for each $\mathcal{O} \in \mathrm{Orb}_G(\mathbb{N}_{r+2-j}^n)$, let

$$\sigma_{\beta_{\mathcal{O}}} = \sum_{\mathcal{I}\in \mathrm{Orb}_{\mathrm{Fix}_G(\beta_{\mathcal{O}})}(\mathbb{N}_j^n)} s_{\mathcal{I}}^{\mathcal{O}} R_{\mathrm{Fix}_G(\beta_{\mathcal{O}})}(x^{\alpha_{\mathcal{I}}^{\mathcal{O}}}) \in \Sigma_j.$$

For any $P \in G$, define $\sigma_{P\beta_{\mathcal{O}}} = \sigma_{\beta_{\mathcal{O}}}(P^\top x)$. Then $\sigma_\beta(x)$ is defined for all β and satisfy conditions (i) and (ii) in Theorem 1, thus $M \in (\mathbb{H}_k^r)^G$. □ □

The main theoretical contribution of having a distinction between outer and inner symmetry is two fold. First the outer symmetry reduction is simple to apply, and produces important reductions in the number of decision variables, the SDP constraint and the linear system. This reduction is analytically given in Theorem 2, and depends only on orbit calculations. Second, the inner symmetry reduction is more complex. Inner symmetry is used to produce a block diagonalization of the SDP constraints, which is not only more computationally involved, but also could be harmful, as could lead to numerical issues and/or huge increase in memory requirement. Having such a distinction allows to obtain important reductions on the dimensionality of the SDP problem given by the outer symmetry, without necessarily applying the block-diagonalization obtained from the inner symmetry reduction.

4 Numerical computations

4.1 Crossing numbers

The crossing number $\mathrm{cr}(G)$ of a graph G is the minimum number of intersections of edges in a drawing of G in the plane. Paul Turán [65] raised the problem of computing the crossing number of the complete bipartite graph $K_{m,n}$.

The crossing number of the complete bipartite graph is known only in a few special cases, such as $\min(m, n) \leq 6$ [29] and $m \leq 8, n \leq 10$ [69]. Zarankiewicz [70], shows well-known upper bound $Z(m, n) = \left\lfloor \frac{m}{2} \right\rfloor \left\lfloor \frac{m-1}{2} \right\rfloor \left\lfloor \frac{n}{2} \right\rfloor \left\lfloor \frac{n-1}{2} \right\rfloor$ on $\mathrm{cr}(K_{m,n})$, which is conjectured to be tight. Therefore, it is interesting to obtain lower bounds on $\mathrm{cr}(K_{m,n})$.

In [31] it is shown how to obtain a lower bound on $\mathrm{cr}(K_{m,n})$ via copositive programming, namely

$$\mathrm{cr}(K_{m,n}) \geq \frac{n}{2}\left(n\theta(m) - \left\lfloor \frac{m}{2} \right\rfloor \left\lfloor \frac{m-1}{2} \right\rfloor\right),$$

where

$$\theta(m) = \min_{X \in \mathcal{C}^*} \{\mathrm{tr}\,(M_m X) : \ \mathrm{tr}\left(J_{(m-1)!} X\right) = 1\} \tag{10}$$

with M_m is a certain (given) matrix of size $(m-1)!$, and $J_{(m-1)!}$ is the all-ones matrix of the same size. The rows and columns of M_m are indexed by all the cyclic orderings of m elements. The cyclic orderings are given by the equivalence classes of orderings that are equal modulo a cyclic permutation. Therefore, we have $\frac{m!}{m}$ cyclic orderings that we denote $u_1, ..., u_{(m-1)!}$. The entries M_{ij} are given by the distance between cyclic orderings u_i and u_j. This distance is given by the number of neighbor swaps needed to go from one ordering to another; for example the distance between 123 and 213 is one.

In [31], the optimization problem in (10) is relaxed, for m =7, to the corresponding problem over $(\mathbb{H}_2^0)^* = \{X \in \mathbb{S} : X \succeq 0,\, X \geq 0\}$. Using simple block-diagonalization techniques (decomposition into two blocks of equal size) for the SDP data the following bound is obtained

$$\mathrm{cr}(K_{7,n}) \geq 2.1796n^2 - 4.5n.$$

The same relaxation is solved for $m = 9$ in [37] using representation theory (regular *-representation of a certain matrix *-algebra) and the following bound is obtained

$$\mathrm{cr}(K_{9,n}) \geq 3.8676063n^2 - 8n.$$

In this paper, we exemplify the importance of exploiting the outer symmetry exhibited by the hierarchy of cones $\mathbb{H}_k^r$ by providing new lower bounds for $\mathrm{cr}(K_{7,n})$.

4.1.1 New lower bounds for cr$(K_{7,n})$

For the case of $\mathrm{cr}(K_{7,n})$, using symmetry reduction, we preprocess and compute the optimal value for the relaxation of the problem (10) over $\mathbb{H}_2^1$, obtaining $\theta(7) \geq 4.4060$. This is an improvement over the previous best known bound $\theta(7) \geq 4.3593$ computed by de Klerk et all. in [31]. From Zarankiewicz $\theta(7) \leq 4.5$. Therefore, we have closed the gap for $\theta(7)$ in at least 33.19% with respect to the best previous bound. The new bound on $\theta(7)$ implies the bound $\mathrm{cr}(K(7,n)) \geq 2.2030n^2 - 4.5n$. The best previously existing lower bound (see [31] and references therein) for $\mathrm{cr}(K(7,n))$ is given by

$$\mathrm{cr}(K(7,n)) \geq \begin{cases} Z(7,n) & \text{if } n \leq 10 \\ 2n(n-1) & \text{if } 11 \leq n \leq 22 \\ 2.1796n^2 - 4.5n & \text{if } 23 \leq n \end{cases}$$

Thus our new bound is the best existing bound for $n \geq 13$. Notice that showing, $\theta(7) = 4.5$ will show $Z(7,n)$ is tight for all even n.

Definition (1) of $\mathbb{H}_2^1$ uses $N = (m-1)! = 720$ SDP matrices of size $N \times N$, plus a linear system of $\binom{N+2}{3} = 62.467.440$ equations. Problem (10) is invariant under the group $\mathcal{A}_7 = \mathrm{Aut}(M_7) := \{P \in \mathcal{P}_n : P^\top M_7 P = M_7\}$. which acts transitively on $\{1, \ldots, N\}$. Using Theorem 2 we build a representation of $(\mathbb{H}_2^1)^{\mathcal{A}_7}$ using one SDP matrix of size $N \times N$, and a linear system with 6.583 (the number of 3-orbits of $\mathcal{A}_7$) equations.

The problem is constructed and solved in less than four hours using MATLAB, YALMIP [43] and SDPT3 [66] in Coral lab at ISE Lehigh University, in a machine with 32 GB of RAM and 16 AMD Opteron 2.0 GHz Processors.

The reduction used here only exploits the outer symmetry, as the inner symmetry group $\mathrm{Fix}_{\mathcal{A}_7}(e_1)$ is too small (has order 14), which makes exploiting this symmetry worthless. On one hand attempting to use the regular *-representation as in [37] yields to an SDP constraint of size 19.305. On the other hand attempting to further block diagonalize the basis of the coherent algebra, as in [45] yields to numerical intractability: while the number of nonzero entries in the coherent configuration (i.e. the basis before block diagonalization) is 720×720, after applying block diagonalization (i.e. using the inner symmetry) the new basis is block diagonal, however the number of nonzero elements increases by a factor of almost 1500.

4.2 Stability number

The stability number $\alpha(G)$ of a graph G is the maximum number of pairwise disjoint vertices of G or equivalently, the maximum size of a *clique* in the complement graph $\overline{G}$.

The following copositive reformulation for the stability number of a graph G with adjacency matrix A is given in [36].

$$\alpha(G) := \max\left\{\lambda : \lambda(A_G + I) - J \in \mathcal{C}\right\}, \tag{11}$$

where A_G is the adjacency matrix of the graph, and I and J are the identity and all-ones matrices of the same size as A_G. Note that the problem (11) is invariant under $\mathrm{Aut}(G)$, the automorphism group of G.

Using (1), for each $k, r \geq 0$, we define the following upper bounds for $\alpha(G)$:

$$\vartheta_k^r(G) := \max\left\{\lambda : \lambda(A_G + I) - J \in \mathbb{H}_k^r\right\}. \tag{12}$$

It can be shown that $\lim_{r\to\infty} \vartheta_k^r(G) = \alpha(G)$, for any $k := k(r) \geq 0$. If G is not a clique, then $\vartheta_0^r(G) > \alpha(G)$ for all r (see [51]). It is an open problem whether for all G there is some r and k such that $\vartheta_k^r(G) = \alpha(G)$. De Klerk and Pasechnik [36] conjecture that $\vartheta_{r+2}^r(G) = \alpha(G)$ for $r \geq \alpha(G)$.

4.2.1 Analytical Expression for Cycles and the Icosahedron

Let C_n be the cycle graph in n vertices and $\bar{C}_n$ its graph-complement. Peña, Vera and Zuluaga in [51] present analytical certificates for $\vartheta_2^0(C_{2m}) = \alpha(C_{2m})$, $\vartheta_2^1(C_{2m+1}) = \alpha(C_{2m+1})$ and $\vartheta_2^1(\bar{C}_{2m+1}) = \alpha(C_{2m+1})$, for all $m \geq 2$. For the case of odd cycles and its complements, the given certificate is of the form

$$(e^\top x)x^\top(\alpha(G)(A_G + I) - J)x = \sum x_i p(x_i, x_{i+1}, \ldots, x_n, x_1, \ldots, x_{i-1}),$$

where $p(x) = s(x) + q(x)$ for some degree-2 SOS $s(x)$ and some degree-2 polynomial $q(x)$ with non-negative coefficients. Notice that these certificates are of the form stated in Theorem 1.

No analytical examples of certificate of optimality for $\theta_k^2(G) = \alpha(G)$ were previously known for graphs for which $\theta_k^1(G) > \alpha(G)$. We present one such a example. Let S_I be the skeleton of the icosahedron. This graph has $n = 12$ vertices and 30 edges (see Figure 1). The automorphism group of this graph has order 120. This graph is vertex-transitive and, even more, distance-transitive. Using the symmetry reduction from Theorem 2 we found numerically that $\vartheta_2^0(S_I) = 3.2361 = \vartheta_2^1(S_I)$ and $\vartheta_2^2(S_I) = 3 = \alpha(S_I)$. We have converted the numerical certificate for $\vartheta_2^2(S_I) = \alpha(S_I)$ into an analytical certificate. This is possible thanks to the simplification of the certificate, due to the outer symmetry.

Lemma 4. *Let A_I be the adjacency matrix of the skeleton of the icosahedron. Then $3(A_I+I)-J \in \mathbb{H}_2^2$.*

Proof. Let $P_I(x) = 3x^\top(A_I + I)x - (e^\top x)^2$. Let $\mathcal{A}_I$ be the automorphism group of S_I. Let

$$\sigma_1(x) = (2x_1 + 2x_2 + 2x_3 + 2x_4 + 2x_5 + 2x_9 - x_6 - x_7 - x_8 - x_{10} - x_{12})^2 + x_{11}^2$$
$$\sigma_2(x) = (2x_1 + 2x_2 - x_8 - x_{10})^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 + x_7^2 + x_9^2$$
$$\sigma_3(x) = x_2^2 + x_5^2 + (x_9 - x_{11})^2 + \frac{9}{4}(x_1 + x_3 + x_4 - x_6 - x_7 - x_{10})^2$$

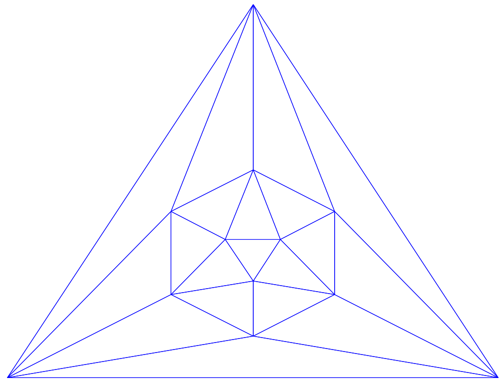

Figure 1: Icosahedron graph

$$+\frac{7}{4}(x_1+x_3+x_4+x_6+x_7+x_{10}-2x_8-2x_{12})^2$$
$$\sigma_4(x)=(x_1-x_{11})^2+(x_2-x_{12})^2+(x_3-x_{10})^2+(x_4-x_7)^2+(x_5-x_8)^2+(x_6-x_9)^2.$$

Then
$$(e^\top x)^2 P_I(x) - R_{\mathcal{A}_I}(6x_1^2\sigma_1(x)+30x_1x_2\sigma_2(x)+30x_1x_6\sigma_3(x)+6x_1x_11\sigma_4(x))$$
has nonnegative coefficients. □

□

4.2.2 Graphs with $\alpha(G) < \vartheta_2^r(G)$ for arbitrary r

Even though it still open whether $\alpha(G) = \vartheta_2^r(G)$ for some r, few graphs are known for which $\vartheta_2^r(G) > \alpha(G)$ for $r \geq 2$. Peña, Vera and Zuluaga [51] construct a family of graphs $\{H_k : k = 1,\ldots,5\}$, the smallest graphs such that $\vartheta_2^{\alpha(H_k)-2}(H_k) > \alpha(H_k) = k+1$, for $k = 1,\ldots,5$. For each k, the graph H_k has $3k+2$ vertices and $\alpha(H_k) = k+1$. These graphs have proven already to be hard test instances for problem (11) [9, 15, 63, 21].

A class $\{G_k : k = 1, 2, \ldots\}$ generalizing the previous construction for all k is conjectured by Peña, Vera and Zuluaga [53] to have the property $\vartheta_2^{\alpha(G_k)-2}(G_k) > \alpha(G_k) = k+1$. The k-th element of the family is constructed as follows: Let $K_{k+1,k+1}$ be the complete bipartite graph with vertex set $\{(-1,i),(1,i) : i = 0,\ldots,k\}$. Let G_k be the graph obtained by adding a vertex to each edge of the form $\{(-1,i),(1,i)\}$ for $i = 1,\ldots,k$. That is k new vertices $\{(0,i) : i = 1,\ldots,k\}$ are added, and for each $i = 1,\ldots,k$ the edge $\{(-1,i),(1,i)\}$ is deleted and the two edges $\{(-1,i),(0,i)\}$ and $\{(0,i),(1,i)\}$ are added (see fig. 2). It is easy to see that $|G_k| = 3k+2$ and that the set $\{(-1,i) : i = 0,\ldots,k\}$ is an independent set of maximal size, i.e. $\alpha(G_k) = k+1$. Peña, Vera and Zuluaga [53] conjecture $\vartheta_2^{k-1}(G_k) > k+1$.

We use Theorem 2 to compute $\vartheta_2^r(G_k)$ for several values of k and $r \leq k+1$. These particular graphs do **not** have a transitive automorphism group for $k > 1$. For this reason the outer symmetry do not reduce (12) to a problem with a single SDP matrix. For any $r \geq 1$. The number of SDP variables goes down from $|\mathbb{N}_r^{3k+2}| = \binom{3k+r+1}{r}$ to the number of $r-orbits$. We do not exploit the inner symmetry to obtain further reductions in size, as each SDP variable is a $3k+2$ by $3k+2$ matrix, which is already small for the cases considered. The number of linear constrains involved in the definition of $\mathbb{H}_2^r$ goes down from $|\mathbb{N}_{r+2}^{3k+2}| = \binom{3k+r+3}{r+2}$ to the number of $(r+2)-orbits$

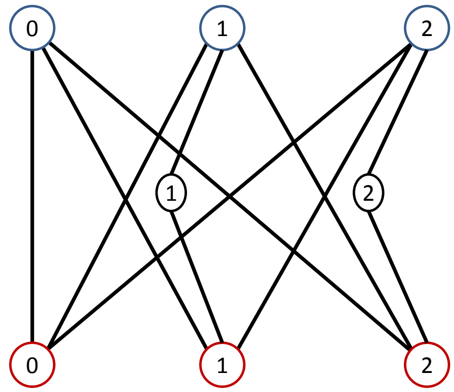

Figure 2: The graph G_2

For each k and $r \leq k+1$, we report in Table 2 (respectively Table 3) the size of the original problem (12) (resp. of the reduced problem). We give the number of SDP matrices and the size of the linear constrains (number of equations × number of variables). We also report the time to construct and to solve the resulting SDP problem without (resp. with) symmetry reduction.

All computations shown in tables 2 and 3 were realized using SDPT3 [66] and YALMIP [43] under Matlab 7.14 (R2012a) on an Intel Core i7 CPU running at 2.3 GHz with 4 KB cache and 3 GB RAM under the Windows 8.1 operating system (64-bit).

For this class of graphs, computing their automorphism group is fast. Using GAP, version 4.4.10 we could compute it for any $k = 1, ..., 7$ in less than one second. Hence we omit this time from the comparison between tables 2 and 3.

For the values of $k = 1, \ldots, 5$ we could apply the reduction to the whole hierarchy (i.e. up to level $r = k$ respectively). The numerical results in the tables show the time advantage of using Theorem 2, both with respect to computing the linear description of the cone $\mathbb{H}^r_k$, and with respect to solving the resulting SDP problem. For several combinations of k and r the optimal value can only computed after symmetry reductions. These optimal values are marked with $*$ in table 3.

If we fail to compute the value of $\vartheta(G_k)^r_2$ we report this with a $-$. In this case the reason for failure is reported as either a "out of memory problem" (MEM) or "8000 seconds time limit reached" (>8000).

We check the conjecture up to $k = 5$. G_4 is the first graph known to be in $\mathbb{H}^4_2 \setminus \mathbb{H}^3_2 = \mathcal{Q}^4 \setminus \mathcal{Q}^3$. Limitations however, come into play when considering G_5. For this case, one can not compute $\vartheta(G_5)^5_2$ even exploiting the symmetry. Still, from [51] it follows that $\vartheta(G_5)^5_2 = 6$, and thus we have checked the conjecture also for this case. The case $k = 6$, $r = 5$ remains still a challenge, and thus the conjecture is not verified for $k = 6$ yet.

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				Time (sec)		Size description of $\mathbb{H}_2^r$	
k	$\|G_k\|$	r	$\vartheta(G_k)_2^r$	Problem Construction	SDP Solution	# SDP matrices	Size of linear constrain
1	5	1	2,0000	0,01	0,47	5	35×125
2	8	1	3,0222	0,04	0,72	8	120×512
	8	2	3,0000	0,26	1,39	36	330×2304
3	11	1	4,0648	0,13	0,86	11	286×1331
	11	2	4,0067	1,62	4,37	66	1001×7986
	11	3	4,0000	20,56	43,96	286	3003×34606
4	14	1	5,1180	0,34	1,44	14	560×2744
	14	2	5,0213	8,01	17,47	105	2380×20580
	14	3	5,0033	187,12	339,46	560	8568×109760
	14	4	**-**	3763,81	**MEM**	2380	27132 ×466480
5	17	1	6,1792	0,83	3,44	17	969×4913
	17	2	6,0446	31,56	71,85	153	4845× 44217
	17	3	**-**	1086,61	**MEM**	969	20349×280041
6	20	1	7,2448	1,84	6,36	20	1540×8000
	20	2	**-**	107,57	**MEM**	210	8855×84000
7	23	1	8,3132	3,73	12,62	23	2300× 12167
	23	2	**-**	**MEM**			

Table 2: Computation results for $\vartheta_2^r(G_k)$ without using symmetry reduction

				Time (sec)		Size desc. $(H_2^r)^{Aut(G_k)}$	
k	$\|G_k\|$	r	$\vartheta(G_k)_2^r$	Problem Construc.	SDP Solution	# SDP matrices	Size of linear constrain
1	5	1	2,0000	0,01	0,45	1	5×9
2	8	1	3,0222	0,03	0,49	3	35×78
	8	2	3,0000	0,13	0,73	13	95×346
3	11	1	4,0648	0,04	0,50	3	41×88
	11	2	4,0067	0,21	0,89	13	125×463
	11	3	4,0000	2,37	4,49	41	331×1829
4	14	1	5,1180	0,05	0,51	3	41×88
	14	2	5,0213	0,29	0,94	13	134×483
	14	3	5,0033	6,71	5,72	41	378×2065
	14	4	***5,0000**	435,71	96,73	134	1034×7708
5	17	1	6,1792	0,06	0,54	3	41×88
	17	2	6,0446	0,53	1,00	13	134×483
	17	3	***6,0106**	19,67	6,68	41	390×2097
	17	4	***6,0020**	2000,07	130,37	134	1103×8109
	17	5	**-**	**>8000**			
6	20	1	7,2448	0,11	1,61	3	41×88
	20	2	***7,0723**	1,59	0,82	13	134×483
	20	3	***7,0232**	60,90	7,42	41	390×2097
	20	4	***7,0066**	7059,60	166,99	134	1119×8157
	20	5	**-**	**MEM**			
7	23	1	8,3132	0,58	0,25	3	41×88
	23	2	***8,1043**	8,77	0,81	13	134×483
	23	3	***8,0390**	234,06	8,59	41	390×2097
	23	4	**-**	**>8000**			

Table 3: Computation results for $\vartheta_2^r(G_k)$ using **outer** symmetry reduction

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