

Semidefinite programming and eigenvalue bounds for the graph partition problem

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Abstract

The graph partition problem is the problem of partitioning the vertex set of a graph into a fixed number of sets of given sizes such that the total weight of edges joining different sets is optimized. In this paper we simplify a known matrix-lifting semidefinite programming relaxation of the graph partition problem for several classes of graphs and also show how to aggregate additional triangle and independent set constraints for graphs with symmetry. We present a closed form expression for the graph partition problem of a strongly regular graph, extending a similar result for the equipartition problem. We also derive a linear programming bound of the graph partition problem for certain Johnson and Kneser graphs. Using what we call the Laplacian algebra of a graph, we derive an eigenvalue bound for the graph partition problem that is the first known closed form bound that is applicable to any graph, thereby extending a well-known result in spectral graph theory. Finally, we strengthen a known semidefinite programming relaxation of a specific quadratic assignment problem and the above-mentioned matrix-lifting semidefinite programming relaxation by adding two constraints that correspond to assigning two vertices of the graph to different parts of the partition. This strengthening performs well on highly symmetric graphs when other relaxations provide weak or trivial bounds.

Keywords: graph partition problem, semidefinite programming, eigenvalues, strongly regular graph, symmetry

1 Introduction

The graph partition problem (GPP) is the problem of partitioning the vertex set of a graph into a fixed number, say k , of sets of given sizes such that the total weight of edges joining different sets is optimized. Here we also refer to the described GPP problem as the k -partition problem. The GPP is a NP-hard combinatorial optimization problem, see [23]. It has many applications such as VLSI design [33], parallel computing [3, 27, 41], network partitioning [21, 40], and floor planing [9]. For recent advances in graph partitioning, we refer to [7].

There are several approaches for deriving bounds for the GPP. Here we are interested in eigenvalue and semidefinite programming (SDP) bounds. Donath and Hoffman [19] derived an eigenvalue-based bound for the GPP that was further improved by Rendl and Wolkowicz [38]. Falkner, Rendl, and Wolkowicz [20] derived a closed form expression for the minimum k -partition problem when $k = 2, 3$ by using the bound from [38]. Their

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bound for $k = 2$ coincides with a well-established result in spectral graph theory; see e.g., Juvan and Mohar [29]. Alizadeh [1] and Karish and Rendl [31] showed that the Donath-Hoffman bound from [19] and the Rendl-Wolkowicz bound from [38], respectively, can be reformulated as semidefinite programs. Other SDP relaxations of the GPP were derived in [31, 47, 30, 13, 43]. For a comparison of all these relaxations, see [42, 43].

Armbruster, Helmberg, Fügenschuh, and Martin [2] evaluated the strength of a branch-and-cut framework for linear and semidefinite relaxations of the minimum graph bisection problem on large and sparse instances. Their results show that in the majority of the cases the semidefinite approach outperforms the linear one. This is very encouraging since SDP relaxations are widely believed to be of use only for instances that are small and dense. The aim of this paper is to further investigate eigenvalue and SDP bounds for the GPP.

Main results and outline

Symmetry in graphs is typically ascribed to symmetry coming from the automorphism group of the graph. However, symmetry may also be interpreted (and exploited) more broadly as what we call combinatorial symmetry. In Section 2 we explain both types of symmetry. In particular, in Section 2.1 we explain symmetry coming from groups, while in Section 2.2 we describe combinatorial symmetry and related coherent configurations. The associated coherent algebra is an algebra that can be exploited in many combinatorial optimization problems, in particular the GPP. In the case that a graph has no (or little) symmetry, one can still exploit the algebraic properties of its Laplacian matrix. For this purpose, we introduce the Laplacian algebra and list its properties in Section 2.3.

In Section 4 we simplify the matrix-lifting SDP relaxation from [43] for different classes of graphs and also show how to aggregate triangle and independent set constraints when possible, see Section 4.1. This approach enables us, for example, to solve the SDP relaxation from [43] with an additional $3\binom{n}{3}$ triangle constraints in less than a second (!) for highly symmetric graphs with $n = 100$ vertices. In Section 4.2 we present a closed form expression for the GPP of a strongly regular graph (SRG). This result is an extension of the result by De Klerk et al. [13, 17] where a closed form expression is derived for the graph equipartition problem for a SRG. In Section 4.2 we also show that for all SRGs except for the pentagon, the bound from [43] does not improve by adding triangle inequalities. In Section 4.3 we derive a linear program for the GPP that is equivalent to the SDP relaxation from [43] when the graph under consideration is a Johnson or Kneser graph on triples.

In Section 5 we derive a closed form eigenvalue bound for the GPP for any, not necessarily highly symmetric, graph. This is the first known closed form bound for the minimum k -partition when $k > 3$ and for the maximum k -partition when $k > 2$ that is applicable to any graph. Our result is a generalization of a well-known result in spectral graph theory for the 2-partition problem to any k -partition problem.

In Section 6.1, we derive a new SDP relaxation for the GPP that is suitable for graphs with symmetry. The new relaxation is a strengthened SDP relaxation of a specific quadratic assignment problem (QAP) by Zhao, Karisch, Rendl, and Wolkowicz [46] by adding two constraints that correspond to assigning two vertices of the graph to different parts of the partition. The new bound performs well on highly symmetric graphs when other SDP relaxations provide weak or trivial bounds. This is probably due to the fact that fixing breaks (some) symmetry in the graph under consideration. Finally, in Section 6.2 we show how to strengthen the matrix-lifting relaxation from [43] by adding a con-

straint that corresponds to assigning two vertices of the graph to different parts of the partition. The new matrix-lifting SDP relaxation is not dominated by the relaxation from [46], or vice versa.

The numerical results in Section 7 present the high potential of the new bounds. None of the presented SDP bounds strictly dominates any of the other bounds for all tested instances. The results indicate that breaking symmetry strengthens the bounds from [43, 46] when the triangle and/or independent set constraints do not (or only slightly) improve the bound from [43]. For the cases that the triangle and/or independent set constraints significantly improve the bound from [43], the fixing approach does not seem to be very effective.

2 Symmetry and matrix algebras

A matrix $*$ -algebra is a set of matrices that is closed under addition, scalar multiplication, matrix multiplication, and taking conjugate transposes. In [24, 12, 14] and others, it was proven that one can restrict optimization of an SDP problem to feasible points in a matrix $*$ -algebra that contains the data matrices of that problem. In particular, the following theorem is proven.

Theorem 1 ([14]). *Let \mathcal{A} denote a matrix $*$ -algebra that contains the data matrices of an SDP problem as well as the identity matrix. If the SDP problem has an optimal solution, then it has an optimal solution in \mathcal{A} .*

When the matrix $*$ -algebra has small dimension, then one can exploit a basis of the algebra to reduce the size of the SDP considerably, see e.g. [12, 13, 16]. In the recent papers [12, 13, 11, 17], the authors considered matrix $*$ -algebras that consist of matrices that commute with a given set of permutation matrices that correspond to automorphisms. Those $*$ -algebras have a basis of 0-1 matrices that can be efficiently computed. However, there exist also such $*$ -algebras that are not coming from permutation groups, but from the ‘combinatorial symmetry’, as we shall see below. We also introduce the Laplacian algebra in order to obtain an eigenvalue bound that is suitable for any graph.

Every matrix $*$ -algebra \mathcal{A} has a canonical block-diagonal structure. This is a consequence of the theorem by Wedderburn [45] that states that there is a $*$ -isomorphism

$$\varphi : \mathcal{A} \longrightarrow \bigoplus_{i=1}^p \mathbb{C}^{n_i \times n_i}.$$

One can exploit a $*$ -isomorphism in order to further reduce the size of an SDP.

2.1 Symmetry from automorphisms

An *automorphism* of a graph $G = (V, E)$ is a bijection $\pi : V \rightarrow V$ that preserves edges, that is, such that $\{\pi(x), \pi(y)\} \in E$ if and only if $\{x, y\} \in E$. The set of all automorphisms of G forms a group under composition; this is called the *automorphism group* of G . The *orbits* of the action of the automorphism group acting on V partition the vertex set V ; two vertices are in the same orbit if and only if there is an automorphism mapping one to the other. The graph G is *vertex-transitive* if its automorphism group acts transitively on vertices, that is, if for every two vertices, there is an automorphism that maps one to the other (and so there is just one orbit of vertices). Similarly, G is *edge-transitive* if its automorphism group acts transitively on edges. Here, we identify the automorphism

group of the graph with the automorphism group of its adjacency matrix. Therefore, if G has adjacency matrix A we will also refer to the automorphism group of the graph as $\text{aut}(A) := \{P \in \Pi_n : AP = PA\}$, where Π_n is the set of permutation matrices of size n .

Assume that \mathcal{G} is a subgroup of the automorphism group of A . Then the centralizer ring (or commutant) of \mathcal{G} , i.e., $\mathcal{A}_{\mathcal{G}} = \{X \in \mathbb{R}^{n \times n} : XP = PX, \forall P \in \mathcal{G}\}$ is a matrix $*$ -algebra that contains A . One may obtain a basis for $\mathcal{A}_{\mathcal{G}}$ from the orbitals (i.e., the orbits of the action of \mathcal{G} on ordered pairs of vertices) of the group \mathcal{G} . This basis, say $\{A_1, \dots, A_r\}$ forms a so-called coherent configuration.

Definition 2 (Coherent configuration). *A set of zero-one $n \times n$ matrices $\{A_1, \dots, A_r\}$ is called a coherent configuration of rank r if it satisfies the following properties:*

- (i) $\sum_{i \in \mathcal{I}} A_i = I$ for some index set $\mathcal{I} \subset \{1, \dots, r\}$ and $\sum_{i=1}^r A_i = J$,
- (ii) $A_i^T \in \{A_1, \dots, A_r\}$ for $i = 1, \dots, r$,
- (iii) There exist p_{ij}^h , such that $A_i A_j = \sum_{h=1}^r p_{ij}^h A_h$ for $i, j \in \{1, \dots, r\}$.

As usual, the matrices I and J here denote the identity matrix and all-ones matrix, respectively. We call $\mathcal{A} := \text{span}\{A_1, \dots, A_r\}$ the associated *coherent algebra*, and this is clearly a matrix $*$ -algebra. Note that in the case that A_1, \dots, A_r are derived as orbitals of the group \mathcal{G} , it follows indeed that $\mathcal{A} = \mathcal{A}_{\mathcal{G}}$. If the coherent configuration is commutative, that is, $A_i A_j = A_j A_i$ for all $i, j = 1, \dots, r$, then we call it a (commutative) *association scheme*. In this case, \mathcal{I} contains only one index, and it is common to call this index 0 (so $A_0 = I$), and $d := r - 1$ the number of classes of the association scheme.

In the case of an association scheme, all matrices can be diagonalized simultaneously, and the corresponding $*$ -algebra has a canonical diagonal structure $\oplus_{j=0}^d \mathbb{C}$. The $*$ -isomorphism φ is then given by $\varphi(A_i) = \oplus_{j=0}^d P_{ji}$, where P_{ji} is the eigenvalue of A_i on the j -th eigenspace. The matrix $P = (P_{ji})$ of eigenvalues is called the *eigenmatrix* or *character table* of the association scheme.

Centralizer rings are typical examples of coherent algebras, but not the only ones. In general, the centralizer ring of the automorphism group of A is not the smallest coherent algebra containing A , even though this is the case for well-known graphs such as the Johnson and Kneser graphs that we will encounter later in this paper. We could say that, in general, the smallest coherent configuration captures more symmetry than that coming from automorphisms of the graph. In this case, we say that there is more combinatorial symmetry.

2.2 Combinatorial symmetry

Let us look at coherent configurations and the combinatorial symmetry that they capture in more detail. One should think of the (non-diagonal) matrices A_i of a coherent configuration as the adjacency matrices of (possibly directed) graphs on n vertices. The diagonal matrices represent the different ‘kinds’ of vertices (so there are $|\mathcal{I}|$ kinds of vertices; these generalize the orbits of vertices under the action of the automorphism group). The non-diagonal matrices A_i represent the different ‘kinds’ of edges and non-edges.

In order to identify the ‘combinatorial symmetry’ in a graph, one has to find a coherent configuration (preferably of smallest rank) such that the adjacency matrix of the graph is in the corresponding coherent algebra \mathcal{A} . As mentioned before, not every coherent configuration comes from the orbitals of a permutation group. Most strongly regular

graphs — a small example being the Shrikhande graph — indeed give rise to such examples. A (simple, undirected, and loopless) κ -regular graph $G = (V, E)$ on n vertices is called *strongly regular* with parameters $(n, \kappa, \lambda, \mu)$ whenever it is not complete or edgeless and every two distinct vertices have λ or μ common neighbors, depending on whether the two vertices are adjacent or not, respectively. If A is the adjacency matrix of G , then this definition implies that $A^2 = \kappa I + \lambda A + \mu(J - I - A)$, which implies furthermore that $\{I, A, J - I - A\}$ is an association scheme. The combinatorial symmetry thus tells us that there is one kind of vertex, one kind of edge, and one kind of non-edge. For the Shrikhande graph, a strongly regular graph with parameters $(16, 6, 2, 2)$ (defined by $V = \mathbb{Z}_4^2$, where two vertices are adjacent if their difference is $\pm(1, 0), \pm(0, 1),$ or $\pm(1, 1)$) however, the automorphism group indicates that there are two kinds of non-edges (depending on whether the two common neighbors of a non-edge are adjacent or not), and in total there are four (not three) orbitals. Doob graphs are direct products of K_4 s and Shrikhande graphs, thus generalizing the Shrikhande graph to association schemes with more classes. In many optimization problems the combinatorial symmetry, captured by the concept of a coherent configuration or association scheme, can be exploited, see Section 4.1 and e.g., [16, 25]. In Section 7.2, we will mention some numerical results for graphs that have more combinatorial symmetry than symmetry coming from automorphisms.

2.3 The Laplacian algebra

Let A be an adjacency matrix of a connected graph G and $L := \text{Diag}(Au_n) - A$ the Laplacian matrix of the graph. We introduce the matrix $*$ -algebra consisting of all polynomials in L , and call this algebra the Laplacian algebra \mathcal{L} . This algebra has a convenient basis of idempotent matrices that are formed from an orthonormal basis of eigenvectors corresponding to the eigenvalues of L . In particular, if the distinct eigenvalues of L are denoted by $0 = \lambda_0 < \lambda_1 < \dots < \lambda_d$, then we let $F_i = U_i U_i^T$, where U_i is a matrix having as columns an orthonormal basis of the eigenspace of λ_i , for $i = 0, \dots, d$. Then $\{F_0, \dots, F_d\}$ is a basis of \mathcal{L} that satisfies the following properties:

- $F_0 = \frac{1}{n}J, \sum_{i=0}^d F_i = I, \sum_{i=0}^d \lambda_i F_i = L$
- $F_i F_j = \delta_{ij} F_i, \forall i, j$
- $F_i = F_i^*, \forall i$.

Note that $\text{tr } F_i = f_i$, the multiplicity of eigenvalue λ_i of L , for all i . Clearly, the operator P , where

$$P(Y) = \sum_{i=0}^d \frac{\text{tr } Y F_i}{f_i} F_i$$

is the orthogonal projection onto \mathcal{L} .

We note that the Laplacian algebra of a strongly regular graph is the same as the corresponding coherent algebra $\text{span}\{I, A, J - I - A\}$ (and a similar identity holds for graphs in association schemes).

3 The graph partition problem

The minimum (resp. maximum) graph partition problem may be formulated as follows. Let $G = (V, E)$ be an undirected graph with vertex set V , where $|V| = n$ and edge set

E , and $k \geq 2$ be a given integer. The goal is to find a partition of the vertex set into k (disjoint) subsets S_1, \dots, S_k of specified sizes $m_1 \geq \dots \geq m_k$, where $\sum_{j=1}^k m_j = n$, such that the total weight of edges joining different sets S_j is minimized (resp. maximized). The case when $k = 2$ is known as the *graph bisection problem* (GBP). If all m_j ($j = 1, \dots, k$) are equal, then we refer to the associated problem as the *graph equipartition problem* (GEP).

We denote by A be the adjacency matrix of G . For a given partition of the graph into k subsets, let $X = (x_{ij})$ be the $n \times k$ matrix defined by

$$x_{ij} = \begin{cases} 1 & \text{if } i \in S_j \\ 0 & \text{otherwise.} \end{cases}$$

Note that the j th column of X is the characteristic vector of S_j . The total weight of edges joining different sets, i.e., the cut of the partition, is equal to $\frac{1}{2} \text{tr} A(J_n - XX^T)$. Thus, the minimum GPP problem can be formulated as

$$\begin{aligned} \min \quad & \frac{1}{2} \text{tr} A(J_n - XX^T) \\ \text{s.t.} \quad & Xu_k = u_n \\ & X^T u_n = m \\ & x_{ij} \in \{0, 1\}, \quad \forall i, j, \end{aligned} \tag{1}$$

where $m = (m_1, \dots, m_k)^T$, and u_k and u_n denote all-ones vectors of sizes k and n , respectively. It is easy to show that if X is feasible for (1), then

$$\frac{1}{2} \text{tr} A(J_n - XX^T) = \frac{1}{2} \text{tr} LXX^T, \tag{2}$$

where L is the Laplacian matrix of the graph. We will use this alternative expression for the objective in Section 5.

4 A simplified and improved SDP relaxation for the GPP

In [43], the second author derived a matrix lifting SDP relaxation for the GPP. Extensive numerical results in [43] show that the matrix lifting SDP relaxation for the GPP provides competitive bounds and is solved significantly faster than any other known SDP bound for the GPP. The goal of this section is to further simplify the mentioned relaxation for highly symmetric graphs. Further, we show here how to aggregate, when possible, certain type of (additional) inequalities to obtain stronger bounds.

The matrix lifting relaxation in [43] is obtained after linearizing the objective function $\text{tr} A(J_n - XX^T)$ by replacing XX^T with a new variable Y , and approximating the set

$$\text{conv} \left\{ XX^T : X \in \mathbb{R}^{n \times k}, Xu_k = u_n, X^T u_n = m, x_{ij} \in \{0, 1\} \right\}.$$

The following SDP relaxation for the GPP is thus obtained.

$$\begin{aligned} \min \quad & \frac{1}{2} \text{tr} A(J_n - Y) \\ \text{s.t.} \quad & \text{diag}(Y) = u_n \\ (\text{GPP}_m) \quad & \text{tr} JY = \sum_{i=1}^k m_i^2 \\ & kY - J_n \succeq 0, \quad Y \geq 0. \end{aligned}$$

We observe the following simplification of the relaxation GPP_m for the bisection problem.

Lemma 3. *For the case of the bisection problem the nonnegativity constraint on the matrix variable in GPP_m is redundant.*

Proof. Let Y be feasible for GPP_m with $k = 2$. We define $Z := 2Y - J_n$. Now from $\text{diag}(Y) = u_n$ it follows that $\text{diag}(Z) = u_n$. Because $Z \succeq 0$, it follows that $-1 \leq z_{ij} \leq 1$, which implies indeed that $y_{ij} \geq 0$. \square

In order to strengthen GPP_m , one can add the triangle constraints

$$y_{ab} + y_{ac} \leq 1 + y_{bc}, \quad \forall(a, b, c). \quad (3)$$

For a given triple (a, b, c) of (distinct) vertices, the constraint (3) ensures that if a and b belong to the same set of the partition and so do a and c , then also b and c do so. There are $3\binom{n}{3}$ inequalities of type (3). For future reference, we refer to $\text{GPP}_{m\Delta}$ as the SDP relaxation that is obtained from GPP_m by adding the triangle constraints.

One can also add to GPP_m and/or $\text{GPP}_{m\Delta}$ the independent set constraints

$$\sum_{a < b, a, b \in W} y_{ab} \geq 1, \quad \text{for all } W \text{ with } |W| = k + 1. \quad (4)$$

These constraints ensure that the graph with adjacency matrix Y has no independent set (W) of size $k + 1$. There are $\binom{n}{k+1}$ inequalities of type (4). For future reference, we refer to $\text{GPP}_{m\text{-ind}}$ as the SDP relaxation that is obtained from GPP_m by adding the independent set constraints.

Constraints (3) and (4) are also used by Karish and Rendl [31] to strengthen the SDP relaxation for the graph equipartition problem, and by the second author [43] to strengthen the SDP relaxation for the (general) graph partition problem. By adding constraints (3) and/or (4) to GPP_m , one obtains — in general — stronger relaxations that are computationally more demanding than GPP_m . In the following sections we will show how to efficiently compute, for graphs with symmetry, all above derived relaxations.

4.1 Symmetry and aggregating triangle and independent set constraints

It is well known how to exploit the symmetry in problems such as GPP_m by using coherent configurations (or association schemes). Aggregating triangle inequalities was suggested by Goemans and Rendl [25] in the context of the maximum cut problem for graphs in association schemes. Surprisingly, the suggestion by Goemans and Rendl was not followed so far in the literature, as far as we know. Here we will extend the approach successfully to coherent configurations. Moreover, we will aggregate the independent set inequalities (4) for the case $k = 2$.

Let us now consider graphs with symmetry, and assume that the data matrices of GPP_m belong to the coherent algebra of a coherent configuration $\{A_1, \dots, A_r\}$. We will first show how this allows us to efficiently solve GPP_m , and subsequently how to aggregate additional triangle and/or independent set constraints.

Because of our assumption, we may consider $Y = \sum_{j=1}^r y_j A_j$ (see Theorem 1) and the

SDP relaxation GPP_m reduces to

$$\begin{aligned}
\min \quad & \frac{1}{2} \text{tr} AJ_n - \frac{1}{2} \sum_{j=1}^r y_j \text{tr} AA_j \\
\text{s.t.} \quad & \sum_{j \in \mathcal{I}} y_j \text{diag}(A_j) = u_n \\
& \sum_{j=1}^r y_j \text{tr} JA_j = \sum_{i=1}^k m_i^2 \\
& k \sum_{j=1}^r y_j A_j - J_n \succeq 0, \quad y_j \geq 0, \quad j = 1, \dots, r,
\end{aligned} \tag{5}$$

where \mathcal{I} is the subset of $\{1, \dots, r\}$ that contains elements of the coherent configuration with nonzero diagonal (as in Definition 2). Note that (5) solves significantly faster than GPP_m when $r \ll n^2/2$. Also, the linear matrix inequality in (5) can be block-diagonalized. In the following sections we will show that the SDP relaxation (5) can be further simplified for some special types of graphs.

Next, we will reduce $\text{GPP}_{m\Delta}$ by adding aggregated triangle inequalities to (5). Because we cannot express a single triangle inequality in terms of the new variables in (5), we consider all inequalities, at once, of the same ‘type’, as follows. For a given triple of distinct vertices (a, b, c) consider the triangle inequality $y_{ab} + y_{ac} \leq 1 + y_{bc}$. If $(A_i)_{ab} = 1$, $(A_h)_{ac} = 1$, and $(A_j)_{bc} = 1$, then we say that this triangle inequality is of type (i, j, h) ($i, j, h \in \{1, \dots, r\} \setminus \mathcal{I}$; note that the indices i, j, h are not necessary distinct). From Definition 2 (iii) it follows that if $(A_i)_{ab} = 1$, then the number of (directed) triangles containing the (directed) edge (a, b) and for which $(A_h)_{ac} = 1$ and $(A_{j'})_{cb}$ is equal to $p_{hj'}^i$ (here j' is the index for which $A_{j'} = A_j^T$). Now, if Y is feasible for (5), then by summing all triangle inequalities of a given type (i, j, h) , the aggregated triangle inequality becomes

$$p_{hj'}^i \text{tr} A_i Y + p_{ij}^h \text{tr} A_h Y \leq p_{hj'}^i \text{tr} A_i J + p_{i'h}^j \text{tr} A_j Y. \tag{6}$$

After exploiting the fact that $Y = \sum_{j=1}^r y_j A_j$, the aggregated inequality (6) reduces to a linear inequality that can be added to the relaxation (5). The number of aggregated triangle inequalities is bounded by r^3 which may be significantly smaller than $3\binom{n}{3}$. So the SDP relaxation $\text{GPP}_{m\Delta}$ can be efficiently computed for small r .

For the bisection problem (i.e., $k = 2$), the independent set constraints (4) can be aggregated in a similar way as the triangle inequalities, and we obtain that

$$p_{hj'}^i \text{tr} A_i Y + p_{ij}^h \text{tr} A_h Y + p_{i'h}^j \text{tr} A_j Y \geq p_{hj'}^i \text{tr} A_i J. \tag{7}$$

It is not clear how to aggregate the independent set constraints for $k \geq 3$. Note that in the case that the considered coherent configuration is an association scheme, all matrices are symmetric which simplifies the above aggregation processes.

4.2 Strongly regular graphs

In this section we show that for a strongly regular graph, the SDP relaxation GPP_m has a closed form expression. A similar approach was used in [13, 17] to derive a closed form expression for the equipartition problem from the SDP relaxation presented by Karish and Rendl [31]. Furthermore, we show that the triangle inequalities are redundant in GPP_m for connected SRGs, except for the pentagon and the complete multipartite graphs.

Let A be the adjacency matrix of a strongly regular graph G with parameters $(n, \kappa, \lambda, \mu)$, see Section 2.2. Using the matrix equation $A^2 = \kappa I + \lambda A + \mu(J - I - A)$, we can determine the eigenvalues of the matrix A from the parameters of G , see e.g., [6]. Since G is regular with valency κ , it follows that κ is an eigenvalue of A with eigenvector u_n . The matrix A has exactly two distinct eigenvalues associated with eigenvectors orthogonal to u_n . These two eigenvalues are known as *restricted eigenvalues* and are usually denoted by $r \geq 0$ and $s < 0$. The character table of the corresponding association scheme is

$$P = \begin{pmatrix} 1 & \kappa & n - 1 - \kappa \\ 1 & r & -1 - r \\ 1 & s & -1 - s \end{pmatrix}. \quad (8)$$

From Theorem 1 it follows that there exists an optimal solution Y to GPP_m in the coherent algebra spanned by $\{I, A, J - A - I\}$. Because of the constraints $\text{diag}(Y) = u_n$ and $Y \geq 0$, there exist $y_1, y_2 \geq 0$ such that

$$Y = I + y_1 A + y_2 (J - A - I), \quad (9)$$

which we shall use to get an even simpler form than (5). The constraint $\text{tr} JY = \sum_{i=1}^k m_i^2$ reduces to

$$n + n\kappa y_1 + (n^2 - n\kappa - n)y_2 = \sum_{i=1}^k m_i^2. \quad (10)$$

Since the matrices $\{I, A, J - A - I\}$ may be simultaneously diagonalized, the constraint $kY - J_n \succeq 0$ becomes a system of linear inequalities in the variables y_1 and y_2 . In particular, after exploiting (8), the constraint $kY - J_n \succeq 0$ reduces to the three constraints

$$k + k\kappa y_1 + k(n - \kappa - 1)y_2 - n \geq 0, \quad (11)$$

$$1 + r y_1 - (r + 1)y_2 \geq 0, \quad (12)$$

$$1 + s y_1 - (s + 1)y_2 \geq 0. \quad (13)$$

Because $\sum_{i=1}^k m_i^2 \geq n^2/k$ by Cauchy's inequality, (11) is actually implied by (10), so we may remove this first constraint. It remains only to rewrite the objective function, i.e.,

$$\frac{1}{2} \text{tr} A(J_n - Y) = \frac{\kappa n(1 - y_1)}{2}.$$

To summarize, the SDP bound GPP_m can be obtained by solving the following linear programming (LP) problem

$$\begin{aligned} \min \quad & \frac{1}{2} \kappa n (1 - y_1) \\ \text{s.t.} \quad & \kappa y_1 + (n - \kappa - 1)y_2 = \frac{1}{n} \sum_{i=1}^k m_i^2 - 1 \\ & 1 + r y_1 - (r + 1)y_2 \geq 0 \\ & 1 + s y_1 - (s + 1)y_2 \geq 0 \\ & y_1 \geq 0, \quad y_2 \geq 0. \end{aligned} \quad (14)$$

It is straightforward to derive a closed form expression for (14) that is given in the following theorem.

Theorem 4. Let $G = (V, E)$ be a strongly regular graph with parameters $(n, \kappa, \lambda, \mu)$ and restricted eigenvalues $r \geq 0$ and $s < 0$. Let k and m_i ($i = 1, \dots, k$) be positive integers such that $\sum_{j=1}^k m_j = n$. Then the SDP bound GPP_m for the minimum GPP of G is given by

$$\max \left\{ \frac{\kappa - r}{n} \sum_{i < j} m_i m_j, \frac{1}{2} \left(n(\kappa + 1) - \sum_i m_i^2 \right) \right\}.$$

Similarly, the SDP bound GPP_m for the maximum GPP is given by

$$\min \left\{ \frac{\kappa - s}{n} \sum_{i < j} m_i m_j, \frac{1}{2} \kappa n \right\}.$$

For the case of the GEP, the results of Theorem 4 coincide with the results from [17] and [13]. To see that, one should use the equation $n(\kappa + rs) = (\kappa - s)(\kappa - r)$ (which follows from taking row sums of the equation $(A - rI)(A - sI) = (\kappa + rs)J$) and other standard equations for the parameters of strongly regular graphs (see e.g., [6]), and the fact that GPP_m is equivalent to the SDP relaxation for the GEP problem by Karish and Rendl [31] (see [43]).

Next, we consider $\text{GPP}_{m\Delta}$ for SRGs. From (6) and (9), with $A_1 := A$ and $A_2 := J - A - I$, it follows that for given $i, j, h \in \{1, 2\}$ the aggregated triangle inequality reduces to

$$(\text{tr } BA)y_1 + (\text{tr } B(J - A - I))y_2 \leq b,$$

where $B = p_{hj}^i A_i + p_{ij}^h A_h - p_{ih}^j A_j$ and $b = p_{hj}^i \text{tr } A_i J$. After simplifying and removing equivalent inequalities, at most the inequalities

$$y_1 \leq 1, \quad y_2 \leq 1, \tag{15}$$

$$1 + y_1 - 2y_2 \geq 0, \tag{16}$$

$$1 - 2y_1 + y_2 \geq 0, \tag{17}$$

remain, and when some of the intersection numbers p_{ij}^h vanish, even fewer remain (we omit details for the sake of readability). It is not hard to see that the constraints (15) are always redundant to the constraints of (14) (for example by drawing the feasible region), and that (16) (cf. (12)) and (17) (cf. (13)) are redundant except for $r < 1$ and $s > -2$, respectively, which occurs only for the pentagon, disconnected SRGS, and complete multipartite graphs. However, for the disconnected SRGs and complete multipartite graphs, the ‘nonredundant’ constraints (16) and (17) (respectively) don’t occur precisely because of the vanishing of the relevant intersection numbers. In other words, adding triangle inequalities to GPP_m for strongly regular graphs does *not* improve the bound, except possibly for the pentagon. On the other hand, if we consider the pentagon and add the triangle inequalities to GPP_m with $m = (2, 3)^T$, then the bound improves and is tight.

For the bisection problem the aggregated independent set constraints are of the form (7), again with $A_1 := A$ and $A_2 := J - A - I$. Our numerical tests show that for many strongly regular graphs, the independent set constraints do not improve GPP_m , but there are also graphs for which $\text{GPP}_{m\text{-ind}}$ dominates GPP_m , see Section 7.4 and 7.5.

4.3 Johnson and Kneser graphs

In this section we show that for the Johnson and Kneser graphs (on triples), the SDP bound GPP_m can be obtained by solving a linear programming problem. We also present

aggregated triangle and independent set inequalities that one may add to GPP_m . The Johnson graphs were also studied by Karloff [32] in the context of the max cut problem, in order to show that it is impossible to add valid linear inequalities to improve the performance ratio for the celebrated Goemans-Williamson approximation algorithm. Our results show that GPP_m improves after adding the independent set constraints.

The Johnson and Kneser graphs are defined as follows. Let Ω be a fixed set of size v and let d be an integer such that $1 \leq d \leq v/2$. The vertices of the Johnson scheme $J(v, d)$ are the subsets of Ω with size d . The adjacency matrices of the association scheme are defined by the size of the intersection of these subsets, in particular $(A_i)_{\omega, \omega'} = 1$ if the subsets ω and ω' intersect in $d - i$ elements, for $i = 0, \dots, d$. We remark that A_1 represents a so-called distance-regular graph G — the *Johnson graph* — and A_i represents being at distance i in G . The *Kneser graph* $K(v, d)$ is the graph with adjacency matrix A_d , that is, two subsets are adjacent whenever they are disjoint. The Kneser graph $K(5, 2)$ is the well-known Petersen graph.

For the case $d = 2$, the Johnson graph is strongly regular and also known as a triangular graph. Consequently the bound GPP_m of $J(v, 2)$ has a closed form expression (apply Theorem 4 with $\kappa = 2(v - 2)$, $r = v - 4$, and $s = -2$). Similarly, the Kneser graph $K(v, 2)$ is strongly regular and the closed form expression for the GPP follows from Theorem 4 with $\kappa = \binom{v}{2} - 1 - 2(v - 2)$, $r = 1$, and $s = 3 - v$.

Here we focus on the next interesting group of Johnson and Kneser graphs, i.e., those on triples ($d = 3$), but we also note that the restriction to the case $d = 3$ is not essential. The eigenvalues (character table) of the Johnson scheme can be expressed in terms of Eberlein polynomials; see Delsarte's thesis [18, Thm. 4.6]. For $d = 3$, the character table is

$$P = \begin{pmatrix} 1 & \theta_0 & \varphi(\theta_0) & \binom{v}{3} - 1 - \theta_0 - \varphi(\theta_0) \\ 1 & \theta_1 & \varphi(\theta_1) & -1 - \theta_1 - \varphi(\theta_1) \\ 1 & \theta_2 & \varphi(\theta_2) & -1 - \theta_2 - \varphi(\theta_2) \\ 1 & \theta_3 & \varphi(\theta_3) & -1 - \theta_3 - \varphi(\theta_3) \end{pmatrix}, \quad (18)$$

where $\varphi(\theta) = \frac{1}{4}(\theta^2 - (v - 2)\theta - 3(v - 3))$, $\theta_0 = 3(v - 3)$, $\theta_1 = 2v - 9$, $\theta_2 = v - 7$, and $\theta_3 = -3$.

Let A_1 denote the adjacency matrix of $J(v, 3)$, and A_3 the adjacency matrix of $K(v, 3)$. We first simplify GPP_m for the case that the graph under consideration is the Johnson graph $J(v, 3)$. From Theorem 1, it follows that there exists an optimal solution Y to GPP_m which belongs to the coherent algebra spanned by $\{I, A_1, A_2, A_3\}$. Thus, there exist $y_1, y_2, y_3 \geq 0$ such that

$$Y = I + y_1 A_1 + y_2 A_2 + y_3 A_3. \quad (19)$$

Now, similar to the case of strongly regular graphs (see also [13, 17]), we can rewrite the objective function and constraints from GPP_m by using (19). The derived LP for the minimum GPP is

$$\begin{aligned} \min \quad & \frac{3}{2} \binom{v}{3} (v - 3) (1 - y_1) \\ \text{s.t.} \quad & A_{eq} y = b_{eq} \\ & A_{neq} y \geq b_{neq} \\ & y \geq 0, \quad y \in \mathbb{R}^3, \end{aligned} \quad (20)$$

where

$$A_{eq} := \left(3(v-3), 3 \binom{v-3}{2}, \binom{v-3}{3} \right), \quad (21)$$

$$A_{neq} := \begin{pmatrix} 2v-9 & \frac{1}{2}(v^2-13v+36) & \frac{1}{2}(-v^2+9v-20) \\ v-7 & -2v+11 & v-5 \\ -3 & 3 & -1 \end{pmatrix}, \quad (22)$$

$$b_{eq} := \frac{1}{n} \sum_{i=1}^k m_i^2 - 1, \quad b_{neq} := -(1, 1, 1)^T, \quad (23)$$

and $n = \binom{v}{3}$ is the number of vertices of $J(v, 3)$. To derive (20) we exploited the fact that the matrices $\{I, A_1, A_2, A_3\}$ may be simultaneously diagonalized and we used the character table (18). Note that the computation time for solving (20) is negligible and does not increase with the order of the Johnson graph.

Theorem 5. *Let $J(v, 3)$ be the Johnson graph, with n vertices, and let k and m_i ($i = 1, \dots, k$) be positive integers such that $\sum_{i=1}^k m_i = n$. Then the SDP bound GPP_m for the minimum GPP of $J(v, 3)$ is equal to the optimal value of the linear programming problem (20).*

Similarly, we simplify GPP_m for the Kneser graph $K(v, 3)$. Clearly, the only difference is the objective function which corresponds to the partition of the Kneser graph. The resulting LP relaxation is

$$\begin{aligned} \min \quad & \frac{1}{2} \binom{v}{3} \binom{v-3}{3} (1 - y_3) \\ \text{s.t.} \quad & A_{eq} y = b_{eq} \\ & A_{neq} y \geq b_{neq} \\ & y \geq 0, \quad y \in \mathbb{R}^3, \end{aligned} \quad (24)$$

where A_{eq} - b_{neq} are as in (21)-(23). This leads to the following result.

Theorem 6. *Let $K(v, 3)$ be the Kneser graph on n vertices, and let k and m_i ($i = 1, \dots, k$) be positive integers such that $\sum_{i=1}^k m_i = n$. Then the SDP bound GPP_m for the minimum GPP of $K(v, 3)$ is equal to the optimal value of the linear programming problem (24).*

We can add to (20) and (24) the aggregated triangle inequalities (6). For given $i, j, h \in \{1, 2, 3\}$, these reduce to

$$(\text{tr } BA_1)y_1 + (\text{tr } BA_2)y_2 + (\text{tr } BA_3)y_3 \leq b,$$

where $B = p_{hj}^i A_i + p_{ij}^h A_h - p_{ih}^j A_j$ and $b = p_{hj}^i \text{tr } A_i J$. After taking into consideration all possible choices of $i, j, h \in \{1, 2, 3\}$, there remain only seven (aggregated) triangle inequalities when $v = 6$ and eleven when $v > 6$. Numerical results indicate that these additional inequalities do not improve the solution obtained by solving (20) and (24).

Since we know how to aggregate the independent set constraints (7) when $k = 2$, we tested the effect on the bound GPP_m of adding these constraints. The numerical results show that the bound may improve, e.g., for the bisection of $J(7, 3)$ with $m = (17, 18)^T$, it improves from 62 to 64.

5 A new eigenvalue bound for the GPP

In this section we present a closed form expression for the GPP for any graph and any $k \geq 2$. To the best of our knowledge, in the literature there are such general closed form expressions for the GPP only for $k = 2$ (see e.g., Juvan and Mohar [29] and Falkner, Rendl, and Wolkowicz [20]) and $k = 3$ (see [20]).

In order to derive the closed form expression for the GPP, we relax several constraints in GPP_m . In particular, we relax $\text{diag}(Y) = u_n$ to $\text{tr} Y = n$ and remove nonnegativity constraints. Moreover, we use (2) to rewrite the objective in terms of the Laplacian matrix L , which leads to the relaxation

$$\begin{aligned} \min \quad & \frac{1}{2} \text{tr} LY \\ \text{s.t.} \quad & \text{tr} Y = n \\ & \text{tr} JY = \sum_{i=1}^k m_i^2 \\ & kY - J_n \succeq 0. \end{aligned} \tag{25}$$

Recall from Section 2.3 that we denote the distinct Laplacian eigenvalues of the graph by $0 = \lambda_0 < \lambda_1 < \dots < \lambda_d$, and their corresponding multiplicities f_i , for $i = 0, \dots, d$, and let $\mathcal{L} = \text{span}\{F_0, \dots, F_d\}$ be the Laplacian algebra of the graph. By Theorem 1, there exists an optimal solution Y to (25) in \mathcal{L} , and therefore we may assume that $Y = \sum_{i=0}^d y_i F_i$, where $y_i \in \mathbb{R}$ ($i = 0, \dots, d$) (as before, these are the new variables). We will exploit this to rewrite (25). The objective is

$$\text{tr} LY = \text{tr} \left(\sum_{i=0}^d \lambda_i F_i \right) \left(\sum_{j=0}^d y_j F_j \right) = \sum_{i=0}^d \lambda_i f_i y_i.$$

The constraint $\text{tr} Y = n$ reduces to $\sum_{i=0}^d f_i y_i = n$, while the constraint $\text{tr} JY = \sum_{i=1}^k m_i^2$ reduces to $y_0 = (\sum_{i=1}^k m_i^2)/n$. It remains only to reformulate the semidefinite constraint:

$$kY - J = k \sum_{i=0}^d y_i F_i - J = \frac{k \sum_{i=1}^k m_i^2 - n^2}{n^2} J + \sum_{i=1}^d y_i F_i \succeq 0.$$

From this, it follows that $y_i \geq 0$. To conclude, the SDP relaxation (25) reduces to

$$\begin{aligned} \min \quad & \frac{1}{2} \sum_{i=1}^d \lambda_i f_i y_i \\ \text{s.t.} \quad & \sum_{i=1}^d f_i y_i = \frac{2}{n} \sum_{i < j} m_i m_j \\ & y_i \geq 0, \quad i = 1, \dots, d. \end{aligned} \tag{26}$$

Theorem 7. *Let G be a graph on n vertices, and let k and m_i ($i = 1, \dots, k$) be positive integers such that $\sum_{i=1}^k m_i = n$. Then the SDP lower bound (25) for the minimum GPP of G is equal to*

$$\frac{\lambda_1}{n} \sum_{i < j} m_i m_j,$$

and the SDP upper bound for the maximum GPP of G that is obtained by replacing \min by \max in (25) is

$$\frac{\lambda_d}{n} \sum_{i < j} m_i m_j.$$

Proof. This follows from (26). □

Our closed form expression for the bisection problem (the case $k = 2$) coincides with a well-known result in spectral graph theory, see [29, 35]. Therefore, Theorem 7 may be seen as a generalization of this result for the 2-partition problem to any k -partition problem. Falkner, Rendl, and Wolkowicz [20] derived a closed form expression for the minimum 3-partition of the form

$$\frac{1}{2}\theta_1\mu_1 + \frac{1}{2}\theta_2\mu_2, \quad (27)$$

where $\mu_{1,2} = (m_1m_2 + m_1m_3 + m_2m_3 \pm \sqrt{m_1^2m_2^2 + m_1^2m_3^2 + m_2^2m_3^2 - nm_1m_2m_3})/n$, and θ_1 and θ_2 are the two smallest nonzero (not necessarily distinct) Laplacian eigenvalues. It is clear that this lower bound coincides with ours when $\theta_1 = \theta_2 (= \lambda_1)$. To the best of our knowledge there is no other closed form expressions for the minimum k -partition problem when $k > 3$, or for the maximum k -partition problem when $k > 2$ that is applicable to any graph. Although the bounds from Theorem 26 are, in general, dominated by the bounds obtained from GPP_m , they may be useful in the theoretical analysis of the GPP and related problems. Still, our numerical results show that for many problems the new eigenvalue bound is equal to GPP_m , see Section 7. We finally remark that for strongly regular graph, the eigenvalue bounds also follow from Theorem 4 because $\lambda_1 = \kappa - r$ and $\lambda_d = \kappa - s$ (indeed, they are even the same unless $\sum_i m_i^2 < \frac{r+1}{n-\kappa+r}n^2$ or $\sum_i m_i^2 < \frac{-s}{\kappa-s}n^2$, respectively). This is related to the fact that the Laplacian algebra and the used coherent algebra are the same for strongly regular graphs.

6 Improved relaxations for the GPP

6.1 An improved relaxation from the quadratic assignment problem

In this section, we derive a new SDP relaxation for the GPP that is obtained by strengthening the SDP relaxation of the more general quadratic assignment problem by Zhao, Karisch, Rendl, and Wolkowicz [46], by adding two constraints that correspond to assigning two vertices of the graph to different parts of the partition. A similar approach was used by the authors [10] to derive the best known bounds for the bandwidth problem of graphs with symmetry. For the equipartition problem, the new relaxation dominates the relaxation for the GEP by De Klerk et al. [13], that is obtained by fixing one vertex of the graph. Our new bound is however not restricted to the equipartition problem, and it is also suitable for graphs with symmetry.

The GPP is a special case of the quadratic assignment problem

$$\min_{X \in \Pi_n} \frac{1}{2} \text{tr} AXBX^T,$$

where A and B are given symmetric $n \times n$ matrices, and Π_n is the set of $n \times n$ permutation matrices. For the graph partition problem, A is the adjacency matrix of the relevant graph G with n vertices, and B is the adjacency matrix of the complete multipartite graph K_{m_1, \dots, m_k} with k classes of sizes m_1, \dots, m_k (with $m_1 + \dots + m_k = n$). For example, for the k -equipartition problem with $n = km$,

$$B := (J_k - I_k) \otimes J_m, \quad (28)$$

(where \otimes is the Kronecker product). In the general case, B has the same block structure, but the sizes m_1, \dots, m_k of the blocks vary. In particular, for the bisection problem with $m = (m_1, m_2)^T$,

$$B := \begin{pmatrix} 0_{m_1 \times m_1} & J_{m_1 \times m_2} \\ J_{m_2 \times m_1} & 0_{m_2 \times m_2} \end{pmatrix}. \quad (29)$$

Now it follows that the following ‘vector-lifting’ SDP relaxation of this particular QAP (see Zhao et al. [46] and Povh and Rendl [36]) is also a relaxation for the GPP:

$$\begin{aligned} \max \quad & \frac{1}{2} \operatorname{tr}(B \otimes A)Y \\ \text{s.t.} \quad & \operatorname{tr}(I_n \otimes E_{jj})Y = 1, \quad \operatorname{tr}(E_{jj} \otimes I_n)Y = 1, \quad j = 1, \dots, n \\ (\text{GPP}_{\text{QAP}}) \quad & \operatorname{tr}(I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y = 0 \\ & \operatorname{tr} JY = n^2 \\ & Y \geq 0, \quad Y \succeq 0, \end{aligned}$$

where (here and below) $E_{ij} = e_i e_j^T$. In [42] (see also [43]) it is proven that for the equipartition problem, the relaxations GPP_{QAP} and GPP_m are equivalent, and in [43] that the first dominates the second for the bisection problem. De Klerk et al. [13] strengthened GPP_{QAP} for the GEP by adding a constraint that corresponds to assigning an arbitrary vertex of the complete multipartite graph to a vertex in the graph.

Here, we extend the approach from [13] (see also [10]) and assign (several times) a pair of vertices of G to an edge in K_{m_1, \dots, m_k} . By symmetry, we have to do this for one pair of vertices in each orbital (recall from Section 2 that the orbitals actually represent the ‘different’ kinds of pairs of vertices; (ordered) edges, and (ordered) nonedges in the graph G). Let us assume that there are t such orbitals \mathcal{O}_h ($h = 1, 2, \dots, t$) of edges and nonedges, and note that for highly symmetric graphs, t is relatively small. We formally state the above idea in the following theorem.

Theorem 8. *Let G be an undirected graph on n vertices with adjacency matrix A , and let \mathcal{O}_h ($h = 1, 2, \dots, t$) be the orbitals of edges and nonedges coming from the automorphism group of G . Let (s_1, s_2) be an arbitrary edge in K_{m_1, \dots, m_k} while (r_{h1}, r_{h2}) is an arbitrary pair of vertices in \mathcal{O}_h ($h = 1, 2, \dots, t$). Let $\Pi_n(h)$ be the set of matrices $X \in \Pi_n$ such that $X_{r_{h1}, s_1} = 1$ and $X_{r_{h2}, s_2} = 1$ ($h = 1, 2, \dots, t$). Then*

$$\min_{X \in \Pi_n} \operatorname{tr} X^T A X B = \min_{h=1, \dots, t} \min_{X \in \Pi_n(h)} \operatorname{tr} X^T A X B.$$

Proof. Similar to the proof of Theorem 10 in [10]. □

Clearly, exploiting this requires solving several SDP (sub)problems. However, if we assign to an edge (s_1, s_2) in K_{m_1, \dots, m_k} a pair of vertices (r_{h1}, r_{h2}) from \mathcal{O}_h ($h = 1, 2, \dots, t$), then we can add to GPP_{QAP} the constraints

$$\operatorname{tr}(E_{s_i, s_i} \otimes E_{r_{hi}, r_{hi}})Y = 1, \quad i = 1, 2.$$

Thus, we obtain several SDP problems of the form

$$\begin{aligned}
\mu^h := \min \quad & \frac{1}{2} \operatorname{tr}(B \otimes A)Y \\
\text{s.t.} \quad & \operatorname{tr}(I_n \otimes E_{jj})Y = 1, \quad \operatorname{tr}(E_{jj} \otimes I_n)Y = 1, \quad j = 1, \dots, n \\
& \operatorname{tr}(E_{s_i, s_i} \otimes E_{r_{hi}, r_{hi}})Y = 1, \quad i = 1, 2 \\
& \operatorname{tr}(I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y = 0 \\
& \operatorname{tr} JY = n^2 \\
& Y \succeq 0, \quad Y \preceq 0,
\end{aligned} \tag{30}$$

where $h = 1, \dots, t$, and the new lower bound for the GPP is

$$\operatorname{GPP}_{\text{fix}} = \min_{h=1, \dots, t} \mu^h.$$

We remark that μ^h is a relaxation that depends on the particular edge (s_1, s_2) (but not on the particular pair $(r_{h1}, r_{h2}) \in \mathcal{O}_h$). However, for the GEP and GBP (but not in general!), the lower bound $\operatorname{GPP}_{\text{fix}}$ is independent of the edge (s_1, s_2) . This is due to the fact that $K_{m, \dots, m}$ and K_{m_1, m_2} are edge-transitive.

The following proposition follows directly from (30).

Corollary 9. *Let (s_1, s_2) be an arbitrary edge in K_{m_1, \dots, m_k} and (r_{h1}, r_{h2}) be an arbitrary pair of vertices in \mathcal{O}_h ($h = 1, 2, \dots, t$). Then the SDP bound $\operatorname{GPP}_{\text{fix}}$ dominates $\operatorname{GPP}_{\text{QAP}}$.*

Similarly, the following corollary for the GEP follows.

Corollary 10. *Consider the equipartition problem. Let (s_1, s_2) be an arbitrary edge in $K_{m, \dots, m}$, and (r_{h1}, r_{h2}) be an arbitrary pair of vertices in \mathcal{O}_h ($h = 1, 2, \dots, t$). Then the SDP relaxation $\operatorname{GPP}_{\text{fix}}$ dominates the SDP relaxation from [13, Eq. 10].*

It is, in general, hard to solve (30) (and thus $\operatorname{GPP}_{\text{fix}}$) for $n \geq 16$, see e.g., [37]. Therefore we need to further exploit the symmetry of K_{m_1, \dots, m_k} (in particular, consider pointwise stabilizers) and the graphs under consideration, see also [10]. We do this by applying the general theory of symmetry reduction to the SDP subproblems (30) in a mechanical way, as described in, e.g., [10, 11, 13, 15]. After symmetry reduction of (30) the largest linear matrix inequality contains matrices of size $3n$ (resp. $2n$) for the GEP (resp. GBP).

Our numerical results show that $\operatorname{GPP}_{\text{fix}}$ can be a significantly stronger bound than GPP_m for highly symmetric graphs (i.e., for which t is very small) and for cases that the bound obtained by solving GPP_m cannot be improved by adding triangle and independent set constraints. This could be a consequence of the fact that (some) symmetry in the graph has been broken.

6.2 An improved matrix-lifting relaxation

Clearly, we can exploit the idea of fixing a pair of vertices in a graph also in the context of the matrix lifting relaxation GPP_m . Assume again that for the given graph G there are t orbitals \mathcal{O}_h ($h = 1, 2, \dots, t$) of edges and nonedges. Now, in order to assign two (arbitrary) vertices $(r_{h1}, r_{h2}) \in \mathcal{O}_h$ of the graph G to two different subsets, we add to GPP_m the constraint

$$\operatorname{tr}(E_{r_{h1}, r_{h2}} + E_{r_{h2}, r_{h1}})Y = 0.$$

Therefore, computing this new lower bound reduces to solving t subproblems of the form

$$\begin{aligned}
\nu_h^* &:= \max \quad \frac{1}{2} \operatorname{tr} A(J_n - Y) \\
&\text{s.t.} \quad \operatorname{diag}(Y) = u_n \\
&\quad \operatorname{tr} JY = \sum_{i=1}^k m_i^2 \\
&\quad \operatorname{tr}(E_{r_{h1}, r_{h2}} + E_{r_{h2}, r_{h1}})Y = 0 \\
&\quad kY - J_n \succeq 0, \quad Y \geq 0,
\end{aligned} \tag{31}$$

($h = 1, \dots, t$). Consequently, the new matrix-lifting lower bound is a minimum over t SDP bounds, i.e.,

$$\min_{h=1, \dots, t} \nu_h^*. \tag{32}$$

The following result follows immediately.

Corollary 11. *The SDP bound (32) dominates GPP_m .*

In order to solve (31) (and thus (32)) we further exploit symmetry in the graphs under consideration in a similar way as described in Section 4.1.

Our numerical results suggest that the new SDP bound (32) is dominated by GPP_{fix} , and also that (32) is not dominated by GPP_{QAP} , or vice versa.

7 Numerical results

In this section we present numerical results for the graph partition problem. In particular, we compare bounds from all the presented relaxations and several relaxations from the literature. All relaxations were solved with SeDuMi [44] using the Yalmip interface [34] on an Intel Xeon X5680, 3.33 GHz dual-core processor with 32 GB memory. To compute orbitals, we used GAP [22].

7.1 Why symmetry?

We first show the importance of exploiting symmetry in graphs, when applicable, in order to compute SDP bounds. In Table 1 we consider the planar unweighted **grid graphs**, where $|V| = \# \text{ rows} \times \# \text{ columns}$. They are generated by the rudy graph generator [39]. Table 1 presents computational times, in seconds, required to solve GPP_m with and without exploiting symmetry (see also Table 3 in [43, online supplement]). The table reads as follows. In the first two columns, the sizes of the graphs and the sizes of the partitions are specified. The third column lists computational times required to solve GPP_m without exploiting symmetry. The fourth column provides the rank of the associated matrix *-algebra that is obtained as the centralizer ring of the automorphism group of the graph, and the last column contains computational times required to solve GPP_m after exploiting symmetry. Note that even though the graphs are not highly symmetric, the reduction in computational times after exploiting symmetry is significant.

Table 1: Computational time (s.) to solve GPP_m for the min 3-partition problem.

$ V $	m^T	no symmetry	r_{aut}	symmetry
9×9	(35, 30, 16)	198.35	861	1.70
10×10	(50, 25, 25)	799.21	1275	3.41

7.2 Combinatorial symmetry vs. group symmetry

In this section we list numerical results for several graphs that have (substantially) more combinatorial symmetry than symmetry coming from the automorphism group. We provide the eigenvalue bound of Theorem 7 and GPP_m for the GEP of those graphs.

Table 2 reads as follows. In the first three columns, we list the graphs, the number of vertices, and the number of parts k of the equipartition, respectively. **Chang3** is one of the strongly regular graphs introduced by Chang [8] (see also [4]). For a description of the Doob graph, see Section 2.2. Graphs **A64v30** and **A64vEnd** are strongly regular graphs with parameters $(64, 18, 2, 6)$ obtained by Haemers and Spence [26], where 30 (resp. End) means that it is the 30th (resp. last) graph in the list, see also <http://www.maths.gla.ac.uk/~es/SRGs/64-18-2-6>. The **design** graph is the bipartite incidence graph of a symmetric 2-(45, 12, 3)-design, see <http://www.maths.gla.ac.uk/~es/polar/45-12-3.36>. In the fourth column of Table 2 we give the eigenvalue lower bound from Theorem 7, while in the fifth column, we list the SDP bound GPP_m . All presented bounds are rounded up to the closest integer. In the last four columns we list the rank of the coherent configuration corresponding to the graph’s combinatorial symmetry, computational times required to solve GPP_m after exploiting its combinatorial symmetry, the rank of the coherent configuration coming from the automorphism group, and the corresponding computational times, respectively. If a graph is strongly regular we do not report the computational time since for such graphs we use the closed form expression from Theorem 4.

Note that **A64vEnd** does not have any symmetry coming from automorphisms, but it has lots of combinatorial symmetry. We remark that the listed graphs are not isolated cases, but only a sample that shows that combinatorial symmetry may differ significantly from group symmetry.

Table 2: Lower bounds and computational times (s.) for the min GEP.

G	n	k	eig	GPP_m	r_{comb}	time	r_{aut}	time
Chang3	28	7	96	126	3	–	14	0.23
A64v30	64	8	448	448	3	–	90	0.61
Doob	64	8	112	160	4	0.34	8	0.41
A64vEnd	64	4	384	384	3	–	–	14.33
design	90	9	360	360	4	0.40	2074	4.56

7.3 The graph equipartition problem

In this section we compare different relaxations for the equipartition problem. We first present results for the **Higman-Sims** graph [28], see Table 3. The **Higman-Sims** graph is a strongly regular graph with parameters $(100, 22, 0, 6)$. The max and min k -equipartition problem for this graph was studied in [13, 17]. Table 3 reads as follows. The first column specifies whether we are solving a minimization or maximization problem, while the second column shows the number of parts k of the equipartition. The third column provides the new eigenvalue bound, see Theorem 7. The fourth column lists GPP_m which is known to be equivalent to GPP_{QAP} for the case of the equipartition (for a proof, see [42, 43]). The fifth column provides bounds obtained by solving the relaxation from [13] (that is, the improved GPP_{QAP} by adding a constraint that corresponds to fixing a vertex in the graph). In the sixth column, we list the bounds obtained by solving GPP_{fix} , see page 16, while the seventh column contains the bounds obtained by solving the SDP relaxation from [17]. The latter relaxation is the ‘level two reformulation-linearization technique-type relaxation for the QAP with an additional linear matrix inequality constraint’, which is known to be at least as strong as GPP_{QAP} . The bounds improve along with increasing complexity of the relaxations; the strongest bound is from [17]. Note however that the bound from [17] is appropriate only for vertex-transitive graphs, while our bounds do not have such a restriction. The last column provides bounds obtained from heuristics that are taken from Table 2 and 3 in [17]. We remark that the SDP bound (32) provides the same bounds as GPP_m for all problems in Table 3.

Table 3: Bounds for the GEP for the **Higman-Sims** graph.

max	k	eig	GPP_m	[13]	GPP_{fix}	[17]	lower bound
	4	1125	1100	1097	1094	1048	1006
	5	1200	1100	1100	1100	1100	1068
min							upper bound
	20	950	950	951	951	975	980
	25	960	960	963	964	1000	1000

In Table 4 we present results for the maximum equipartition problem for several Johnson and Kneser graphs (see Section 4.3). The table reads as follows. In the first column we list the graphs, in the second column the number of vertices, and in the third column the number of parts k of the equipartition. In the fourth and fifth column we list the new eigenvalue bound and GPP_m , respectively. We do not report computational times for these two bounds since they are obtained from closed form expressions or very small linear programming problems, see Sections 4.2, 4.3, and 5. In the last two columns of Table 4 we list GPP_{fix} and the corresponding required computational times. Since adding triangle inequalities to GPP_m for the problems in Table 4 do not improve GPP_m , we did not make a separate column for $\text{GPP}_{m\Delta}$. All presented bounds are rounded down to the closest integer.

The results show that the new bound GPP_{fix} can be significantly stronger than GPP_m , in particular for problems when the eigenvalue bound and GPP_m provide the same bound. The results also show that the eigenvalue bound performs well for most of the instances.

Table 4: Upper bounds and computational times (s.) for the max GEP.

G	n	k	eig	GPP_m	GPP_{fix}	time
$K(8, 2)$	28	4	210	210	204	7.66
$K(9, 2)$	36	3	324	324	317	14.43
$K(9, 2)$	36	12	444	378	378	5.32
$K(12, 2)$	66	6	1485	1485	1473	31.79
$J(8, 3)$	56	4	378	378	377	148.54
$K(9, 3)$	84	3	840	840	828	551.99
$K(15, 2)$	105	5	3780	3780	3772	106.97
$K(10, 3)$	120	3	2000	2000	1979	1097.10

7.4 The graph bisection problem

In this section we present numerical results for the graph bisection problem. All graphs in Table 5 are strongly regular. The table reads as follows. In the first column we list the graphs. The Johnson graphs are defined in Section 4.3, whereas the Hoffman–Singleton (HS) graph, the Gewirtz graph, and the M_{22} graph are the unique strongly regular graphs with parameters $(50, 7, 0, 1)$, $(56, 10, 0, 2)$, and $(77, 16, 0, 4)$, respectively. In the second column of Table 5 we list the number of vertices in the corresponding graph, while the third column contains the sizes of the subsets. We choose these sizes arbitrarily. In the remaining columns we provide the lower bounds GPP_m , (32), GPP_{QAP} , $\text{GPP}_{m\text{-ind}}$, and GPP_{fix} , respectively. All bounds are rounded up to the closest integer. In Table 6 we provide computational times required to solve the problems from Table 5 (the times to compute GPP_{fix} and (32) are sums of computational times of all subproblems needed to obtain the bounds).

From Table 5 it follows that (32) is not dominated by GPP_{QAP} , or vice versa. Similarly, we may conclude that GPP_{QAP} and GPP_{fix} are not dominated by $\text{GPP}_{m\text{-ind}}$, or vice versa. One more interesting observation is that for all tested instances, the new eigenvalue bound is equal to the bound obtained by solving GPP_m .

Table 5: Lower bounds for the min GBP.

G	n	m^T	GPP_m	(32)	GPP_{QAP}	$\text{GPP}_{m\text{-ind}}$	GPP_{fix}
$J(6, 2)$	15	(8,7)	23	23	23	26	24
$J(7, 2)$	21	(12,9)	36	37	36	38	38
$J(9, 2)$	36	(26,10)	65	66	65	65	67
HS	50	(46,4)	19	19	19	19	21
Gewirtz	56	(53,3)	23	23	24	23	26
$J(12, 2)$	66	(33,33)	198	199	198	198	199
M_{22}	77	(74,3)	41	41	42	41	44
$J(15, 2)$	105	(85,20)	243	243	243	243	246

Table 6: Computational times (s.) for the min GBP.

G	n	(32)	GPP_{QAP}	$\text{GPP}_{\text{m-ind}}$	GPP_{fix}
$J(6, 2)$	15	0.42	0.20	0.17	2.30
$J(7, 2)$	21	0.66	0.23	0.18	2.70
$J(9, 2)$	36	1.06	0.48	0.23	5.21
HS	50	0.68	0.62	0.30	6.58
Gewirtz	56	1.67	1.66	0.34	15.87
$J(12, 2)$	66	1.02	0.95	0.34	8.87
M_{22}	77	1.55	3.15	0.30	19.12
$J(15, 2)$	105	2.27	3.41	0.54	29.19

7.5 Aggregated triangle and independent set constraints

In Section 4.1 we showed how to aggregate triangle and independent set constraints for the case that the data matrices of GPP_m belong to a coherent algebra, and that this is efficient when the rank of this algebra is small. In this section we provide numerical results for graphs whose adjacency matrices indeed belong to a coherent algebra of small rank. In particular, besides the Johnson graph $J(7, 2)$, we consider the distance-regular Pappus, Desargues, Foster, and Biggs-Smith graphs (see [5]), as well as the Dyck graph (the graph on the triangles of the Shrikhande graph, where two triangles are adjacent if they share an edge). In the third column of Table 7, we list the rank of the smallest coherent configuration containing the corresponding adjacency matrix (i.e., coming from the combinatorial symmetry). In all cases, this coherent configuration is the same as the one coming from the automorphism group. In columns five to eight, we list bounds obtained by solving GPP_m , $\text{GPP}_{\text{m}\Delta}$, $\text{GPP}_{\text{m-ind}}$, and GPP_m with (aggregated) triangle and independent set inequalities, respectively. The numerical results in [43] show that to solve $\text{GPP}_{\text{m}\Delta\text{-ind}}$ for a graph without symmetry and $n = 100$ takes more than 3 hours. However, each bound presented in Table 7 is computed in less than a second.

The results show that, for most of the cases, adding triangle inequalities to GPP_m increases the bound more than adding the independent set inequalities to GPP_m . Note that $J(7, 2)$ is a strongly regular graph for which GPP_m improves after adding all independent set constraints.

Table 7: Lower bounds for the min GBP.

G	n	r_{aut}	m^{T}	GPP_m	$\text{GPP}_{\text{m}\Delta}$	$\text{GPP}_{\text{m-ind}}$	$\text{GPP}_{\text{m}\Delta\text{-ind}}$
Pappus	18	5	(10, 8)	6	7	7	7
Desargues	20	6	(15, 5)	4	5	4	5
$J(7, 2)$	21	3	(11, 10)	37	37	40	40
Dyck	32	10	(16, 16)	7	8	7	8
Foster	90	9	(45, 45)	13	18	14	19
Biggs-Smith	102	8	(70, 32)	10	15	10	15

In Table 8, we also list the eigenvalue bound, (32), GPP_{QAP} , and GPP_{fix} for the same

problems as in Table 7. Due to memory restrictions, we couldn't compute GPP_{fix} for the Foster and Biggs-Smith graph. For these graphs, we computed (32) without exploiting their symmetry. The results show that in all cases the eigenvalue bound coincides with GPP_m . The results also show that GPP_{QAP} equals GPP_m in all cases except for the Desargues graph, and that for the listed graphs fixing edges does not improve GPP_m and/or GPP_{QAP} while adding triangle and/or independent set constraints does.

Table 8: Lower bounds for the min GBP.

G	m^T	eig	(32)	GPP_{QAP}	GPP_{fix}
Pappus	(10, 8)	6	6	6	6
Desargues	(15, 5)	4	4	5	6
$J(7, 2)$	(11, 10)	37	38	37	38
Dyck	(16, 16)	7	7	7	7
Foster	(45, 45)	13	13	13	–
Biggs-Smith	(70, 32)	10	10	10	–

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