Comput Optim Appl (2016) 63:333–364
DOI 10.1007/s10589-015-9779-8

Eigenvalue, quadratic programming, and semidefinite programming relaxations for a cut minimization problem

Ting Kei Pong[1] · Hao Sun[2] · Ningchuan Wang[2] · Henry Wolkowicz[2]

Received: 20 January 2014 / Published online: 21 August 2015

Abstract We consider the problem of partitioning the node set of a graph into k sets of given sizes in order to *minimize the cut* obtained using (removing) the kth set. If the resulting cut has value 0, then we have obtained a vertex separator. This problem is closely related to the graph partitioning problem. In fact, the model we use is the same as that for the graph partitioning problem except for a different *quadratic* objective function. We look at known and new bounds obtained from various relaxations for this NP-hard problem. This includes: the standard eigenvalue bound, projected eigenvalue bounds using both the adjacency matrix and the Laplacian, quadratic programming (QP) bounds based on recent successful QP bounds for the quadratic assignment problems, and semidefinite programming bounds. We include numerical tests for large and *huge* problems that illustrate the efficiency of the bounds in terms of strength and time.

Presented at Retrospective Workshop on Discrete Geometry, Optimization and Symmetry, November 24–29, 2013, Fields Institute, Toronto, Canada.

✉ Henry Wolkowicz
hwolkowicz@uwaterloo.ca

Ting Kei Pong
tk.pong@polyu.edu.hk

Hao Sun
hao_sun@live.com

Ningchuan Wang
wangningchuan1987@hotmail.com

[1] Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong

[2] Department of Combinatorics and Optimization, University of Waterloo, Waterloo, ON N2L 3G1, Canada

Keywords Vertex separators · Eigenvalue bounds · Semidefinite programming bounds · Graph partitioning · Large scale

Mathematics Subject Classification 05C70 · 15A42 · 90C22 · 90C27 · 90C59

1 Introduction

We consider a special type of *minimum cut problem, MC*. The problem consists in partitioning the node set of a graph into k sets of given sizes in order to *minimize the cut* obtained by removing the kth set. This is achieved by minimizing the number of edges connecting distinct sets after removing the kth set, as described in [22]. This problem arises when finding a re-ordering to bring the sparsity pattern of a large sparse positive definite matrix into a block-arrow shape so as to minimize fill-in in its Cholesky factorization. The problem also arises as a subproblem of the *vertex separator problem, VS*. In more detail, a vertex separator is a set of vertices whose removal from the graph results in a disconnected graph with $k-1$ components. A typical VS problem has $k=3$ on a graph with n nodes, and it seeks a vertex separator which is optimal subject to some constraints on the partition size. This problem can be solved by solving an MC for each possible partition size. Since there are at most $\binom{n-1}{2}$ 3-tuple integers that sum up to n, and it is known that VS is NP-hard in general [16,22], we see that MC is also NP-hard when $k \geq 3$.

Our MC problem is closely related to the *graph partitioning problem, GP*, which is also NP-hard; see the discussions in [16]. In both problems one can use a model with a *quadratic* objective function over the set of *partition matrices*. The model we use is the same as that for GP except that the quadratic objective function is different. We study both existing and new bounds and provide both theoretical properties and empirical results. Specifically, we adapt and improve known techniques for deriving lower bounds for GP to derive bounds for MC. We consider eigenvalue bounds, a convex quadratic programming, QP, lower bound, as well as lower bounds based on semidefinite programming, SDP, relaxations.

We follow the approaches in [12,21,22] for the eigenvalue bounds. In particular, we replace the standard quadratic objective function for GP, e.g., [12,21] with that used in [22] for MC. It is shown in [22] that one can equally use either the adjacency matrix A or the negative Laplacian $(-L)$ in the objective function of the model. We show in fact that one can use $A - \mathrm{Diag}(d), \forall d \in \mathbb{R}^n$, in the model, where $\mathrm{Diag}(d)$ denotes the diagonal matrix with diagonal d. However, we emphasize and show that this is no longer true for the eigenvalue bounds and that using $d = 0$ is, empirically, stronger. Dependence of the eigenvalue lower bound on diagonal perturbations was also observed for the quadratic assignment problem, QAP, and GP, see e.g., [10,20]. In addition, we find a new projected eigenvalue lower bound using A that has three terms that can be found explicitly and efficiently. We illustrate this empirically on large and huge scale sparse problems.

Next, we extend the approach in [1,2,5] from the QAP to MC. This allows for a QP bound that is based on SDP duality and that can be solved efficiently. The discussion and derivation of this lower bound is new even in the context of GP. Finally, we follow

and extend the approach in [28] and derive and test SDP relaxations. In particular, we answer a question posed in [28] about redundant constraints. This new result simplifies the SDP relaxations even in the context of GP.

1.1 Outline

We continue in Sect. 2 with preliminary descriptions and results on our special MC. This follows the approach in [22]. In Sect. 3 we outline the basic eigenvalue bounds and then the projected eigenvalue bounds following the approach in [12,21]. Theorem 3.7 includes the projected bounds along with our new three part eigenvalue bound. The three part bound can be calculated explicitly and efficiently by finding $k-1$ eigenvalues and two minimal scalar products. The QP bound is described in Sect. 4. The SDP bounds are presented in Sect. 5.

Upper bounds using feasible solutions are given in Sect. 6. Our numerical tests are in Sect. 7. Our concluding remarks are in Sect. 8.

2 Preliminaries

We are given an undirected graph $\mathsf{G} = (N, E)$ with a nonempty node set $N = \{1, \ldots, n\}$ and a nonempty edge set E. In addition, we have a positive integer vector of set sizes $m = (m_1, \ldots, m_k)^T \in \mathbb{Z}^k_+, k > 2$, such that the sum of the components $m^T e = n$. Here e is the vector of ones of appropriate size. Further, we let $\mathrm{Diag}(v)$ denote the diagonal matrix formed using the vector v; the adjoint $\mathrm{diag}(Y) = \mathrm{Diag}^*(Y)$ is the vector formed from the diagonal of the square matrix Y. We let $\mathrm{ext}(K)$ represent the extreme points of a convex set K. We let $x = \mathrm{vec}(X) \in \mathbb{R}^{nk}$ denote the vector formed (columnwise) from the matrix X; the adjoint and inverse is $\mathrm{Mat}(x) \in \mathbb{R}^{n\times k}$. We also let $A \otimes B$ denote the Kronecker product; and $A \circ B$ denote the Hadamard product.

We let

$$P_m := \{S = (S_1, \ldots, S_k) : S_i \subset N, |S_i| = m_i, \forall i, \\ S_i \cap S_j = \emptyset, \forall i \neq j, \ \cup_{i=1}^k S_i = N\}$$

denote the set of all *partitions of* N with the appropriate sizes specified by m. The partitioning is encoded using an $n \times k$ *partition matrix* $X \in \mathbb{R}^{n\times k}$ where the column $X_{:j}$ is the incidence vector for the set S_j

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

Therefore, the set cardinality constraints are given by $X^T e = m$; while the constraints that each vertex appears in exactly one set is given by $Xe = e$.

The set of partition matrices is denoted by $\mathcal{M}_m$. It can be represented using various linear and quadratic constraints. We present several in the following. In particular, we

phrase the linear equality constraints as quadratics for use in the Lagrangian relaxation below in Sect. 5.

Definition 2.1 We denote the set of zero-one, nonnegative, linear equalities, doubly stochastic type, m-diagonal orthogonality type, e-diagonal orthogonality type, and gangster constraints as, respectively,

$$\begin{aligned}
\mathcal{Z} &:= \{X \in \mathbb{R}^{n\times k} : X_{ij} \in \{0,1\}, \forall ij\} = \{X \in \mathbb{R}^{n\times k} : \left(X_{ij}\right)^2 = X_{ij}, \forall ij\} \\
\mathcal{N} &:= \{X \in \mathbb{R}^{n\times k} : X_{ij} \geq 0, \forall ij\} \\
\mathcal{E} &:= \{X \in \mathbb{R}^{n\times k} : Xe = e, X^T e = m\} \\
&= \{X \in \mathbb{R}^{n\times k} : \|Xe - e\|^2 + \|X^T e - m\|^2 = 0\} \\
\mathcal{D} &:= \{X \in \mathbb{R}^{n\times k} : X \in \mathcal{E} \cap \mathcal{N}\} \\
\mathcal{D}_O &:= \{X \in \mathbb{R}^{n\times k} : X^T X = \mathrm{Diag}(m)\} \\
\mathcal{D}_e &:= \{X \in \mathbb{R}^{n\times k} : \mathrm{diag}(XX^T) = e\} \\
\mathcal{G} &:= \{X \in \mathbb{R}^{n\times k} : X_{:i} \circ X_{:j} = 0, \forall i \neq j\}
\end{aligned}$$

There are many equivalent ways of representing the set of all partition matrices. Following are a few.

Proposition 2.2 *The set of partition matrices in $\mathbb{R}^{n\times k}$ can be expressed as the following.*

$$\begin{aligned}
\mathcal{M}_m &= \mathcal{E} \cap \mathcal{Z} \\
&= \mathrm{ext}(\mathcal{D}) \\
&= \mathcal{E} \cap \mathcal{D}_O \cap \mathcal{N} \\
&= \mathcal{E} \cap \mathcal{D}_O \cap \mathcal{D}_e \cap \mathcal{N} \\
&= \mathcal{E} \cap \mathcal{Z} \cap \mathcal{D}_O \cap \mathcal{G} \cap \mathcal{N}.
\end{aligned} \tag{2.1}$$

Proof The first equality follows immediately from the definitions. The second equality follows from the transportation type constraints and is a simple consequence of Birkhoff and Von Neumann theorems that the extreme points of the set of doubly stochastic matrices are the permutation matrices, see e.g., [23]. The third equality is shown in [22, Proposition 1]. The fourth and fifth equivalences contain redundant sets of constraints. □

We let $\delta(S_i, S_j)$ denote the set of edges between the sets of nodes S_i, S_j, and we denote the set of edges with endpoints in distinct partition sets $S_1, \ldots, S_{k-1}$ by

$$\delta(S) = \cup_{i<j<k} \delta(S_i, S_j). \tag{2.2}$$

The minimum of the cardinality $|\delta(S)|$ is denoted

$$\mathrm{cut}(m) = \min\{|\delta(S)| : S \in P_m\}. \tag{2.3}$$

The graph G has a *vertex separator* if there exists an $S \in P_m$ such that the removal of set S_k and its associated edges means that the induced subgraph has no edges across S_i and S_j for any $1 \le i < j \le k-1$. This is equivalent to $\delta(S) = \emptyset$, i.e., $\text{cut}(m) = 0$. Otherwise, $\text{cut}(m) > 0$.[1]

We define the $k \times k$ matrix

$$B := \begin{bmatrix} ee^T - I_{k-1} & 0 \\ 0 & 0 \end{bmatrix} \in \mathcal{S}^k,$$

where $\mathcal{S}^k$ denotes the vector space of $k \times k$ symmetric matrices equipped with the trace inner-product, $\langle S, T \rangle = \text{trace } ST$. We let A denote the adjacency matrix of the graph and let $L := \text{Diag}(Ae) - A$ be the Laplacian.

In [22, Proposition 2], it was shown that $|\delta(S)|$ can be represented in terms of a quadratic function of the partition matrix X, i.e., as $\frac{1}{2}\text{trace}(-L)XBX^T$ and $\frac{1}{2}\text{trace } AXBX^T$, where we note that the two matrices A and $-L$ differ only on the diagonal. From their proof, it is not hard to see that their result can be slightly extended as follows.

Proposition 2.3 *Let $S \in P_m$ be a partition and let $X \in \mathcal{M}_m$ be the associated partition matrix. Then*

$$|\delta(S)| = \frac{1}{2}\text{trace}\,(A - \text{Diag}(d))\,XBX^T, \quad \forall d \in \mathbb{R}^n. \tag{2.4}$$

In particular, setting $d = 0$, Ae, respectively yields $A, -L$.

Proof The result for the choices of $d = 0$, Ae, equivalently $A, -L$, respectively, was proved in [22, Proposition 2]. Moreover, as noted in the proof of [22, Proposition 2], $\text{diag}(XBX^T) = 0$. Consequently,

$$\frac{1}{2}\text{trace } AXBX^T = \frac{1}{2}\text{trace}\,(A - \text{Diag}(d))\,XBX^T, \quad \forall d \in \mathbb{R}^n.$$

In this paper we focus on the following problem given by (2.3) and (2.4):

$$\begin{array}{rl} \text{cut}(m) = \min & \frac{1}{2}\text{trace}(A - \text{Diag}(d))XBX^T \\ \text{s.t.} & X \in \mathcal{M}_m; \end{array} \tag{2.5}$$

here $d \in \mathbb{R}^n$. For simplicity we write $G = G(d) = A - \text{Diag}(d)$ for $d \in \mathbb{R}^n$, and simply use G when no confusion arises. We recall that if $\text{cut}(m) = 0$, then we have obtained a vertex separator, i.e., removing the kth set results in a graph where the first $k-1$ sets are disconnected. On the other hand, if we find a positive lower bound $\text{cut}(m) \ge \alpha > 0$, then no vertex separator can exist for this m. This observation can be employed in solving some classical vertex separator problems that look for

[1] A discussion of the relationship of $\text{cut}(m)$ with the bandwidth of the graph is given in e.g., [8,18,22]. Particularly, for $k = 3$, if $\text{cut}(m) > 0$, then $m_3 + 1$ is a lower bound for the bandwidth.

an *optimal* vertex separator in the case that $k = 3$ with constraints on (m_1, m_2, m_3). Specifically, since there are at most $\binom{n-1}{2}$ 3-tuple integers summing up to n, one only needs to consider at most $\binom{n-1}{2}$ different MC problems in order to find the *optimal* vertex separator.

Though any choice of $d \in \mathbb{R}^n$ is equivalent for (2.5) on the feasible set $\mathcal{M}_m$, as we see repeatedly throughout the paper, this does *not* mean that they are equivalent on the relaxations that we consider. For similar observations concerning diagonal perturbation for the QAP, the GP and their relaxations, see e.g., [10,20]. Finally, note that the feasible set of (2.5) is the same as that of the GP; see e.g., [21,28] for the projected eigenvalue bound and for the SDP bound, respectively. Thus, the techniques for deriving bounds for MC can be adapted to obtain new results concerning lower bounds for GP.

3 Eigenvalue based lower bounds

We now present bounds on $\text{cut}(m)$ based on $X \in \mathcal{D}_O$, the m-diagonal orthogonality type constraint $X^T X = \text{Diag}(m)$. For notational simplicity we define $M := \text{Diag}(m)$, $\tilde{m} := \left(\sqrt{m_1}, \ldots, \sqrt{m_k}\right)^T$ and $\tilde{M} := \text{Diag}(\tilde{m})$. For a real symmetric matrix $C \in \mathcal{S}^t$, we let

$$\lambda_1(C) \geq \lambda_2(C) \geq \cdots \geq \lambda_t(C)$$

denote the eigenvalues of C in nonincreasing order, and set $\lambda(C) = (\lambda_i(C)) \in \mathbb{R}^t$.

3.1 Basic eigenvalue lower bound

The Hoffman–Wielandt bound [14] can be applied to get a simple eigenvalue bound. In this approach, we solve the relaxed problem

$$\begin{array}{rl} \text{cut}(m) \geq \min & \frac{1}{2} \text{trace } GXBX^T \\ \text{s.t.} & X \in \mathcal{D}_O, \end{array} \tag{3.1}$$

where we recall that $G = G(d) = A - \text{Diag}(d)$, $d \in \mathbb{R}^n$. We first introduce the following definition.

Definition 3.1 For two vectors $x, y \in \mathbb{R}^n$, the minimal scalar product is defined by

$$\langle x, y \rangle_- := \min \left\{ \sum_{i=1}^n x_{\phi(i)} y_i : \phi \text{ is a permutation on } N \right\}.$$

In the case when y is sorted in an increasing order, i.e., $y_1 \leq y_2 \leq \cdots \leq y_n$, from the renowned rearrangement inequality, the permutation that attains the minimum above is the one that sorts x in a decreasing order. This fact is used repeatedly in this paper.

We also need the following two auxiliary results.

Theorem 3.2 (Hoffman and Wielandt [14]) *Let C and D be symmetric matrices of orders n and k, respectively, with $k \le n$. Then*

$$\min\left\{\text{trace } CXDX^T : X^TX = I_k\right\} = \left\langle \lambda(C), \begin{pmatrix}\lambda(D)\\ 0\end{pmatrix}\right\rangle_{-}. \tag{3.2}$$

The minimum on the left is attained for $X = \left[p_{\phi(1)} \ldots p_{\phi(k)}\right] Q^T$, where $p_{\phi(i)}$ is a normalized eigenvector to $\lambda_{\phi(i)}(C)$, the columns of $Q = \left[q_1 \ldots q_k\right]$ consist of the normalized eigenvectors q_i of $\lambda_i(D)$, and ϕ is the permutation of $\{1, \ldots, n\}$ attaining the minimum in the minimal scalar product.

Lemma 3.3 [22, Lemma 4] *The k-ordered eigenvalues of the matrix $\tilde{B} := \tilde{M}B\tilde{M}$ satisfy*

$$\lambda_1(\tilde{B}) > 0 = \lambda_2(\tilde{B}) > \lambda_3(\tilde{B}) \ge \cdots \ge \lambda_{k-1}(\tilde{B}) \ge \lambda_k(\tilde{B}). \qquad \square$$

We now present the basic eigenvalue lower bound, which turns out to always be negative.

Theorem 3.4 *Let $d \in \mathbb{R}^n$, $G = A - \text{Diag}(d)$. Then*

$$\text{cut}(m) \ge 0 > p^*_{eig}(G)$$

where

$$p^*_{eig}(G) := \frac{1}{2}\left\langle \lambda(G), \begin{pmatrix}\lambda(\tilde{B})\\ 0\end{pmatrix}\right\rangle_{-} = \frac{1}{2}\left(\sum_{i=1}^{k-2} \lambda_{k-i+1}(\tilde{B})\lambda_i(G) + \lambda_1(\tilde{B})\lambda_n(G)\right).$$

Moreover, the function $p^*_{eig}(G(d))$ is concave as a function of $d \in \mathbb{R}^n$.

Proof We use the substitution $X = Z\tilde{M}$, i.e., $Z = X\tilde{M}^{-1}$, in (3.1). Then the constraint on X implies that $Z^TZ = I$. We now solve the equivalent problem to (3.1):

$$\begin{array}{ll}\min & \frac{1}{2}\,\text{trace } GZ(\tilde{M}B\tilde{M})Z^T\\ \text{s.t.} & Z^TZ = I.\end{array} \tag{3.3}$$

The optimal value is obtained using the minimal scalar product of eigenvalues as done in the Hoffman–Wielandt result, Theorem 3.2. From this we conclude immediately that $\text{cut}(m) \ge p^*_{eig}(G)$. Furthermore, the explicit formula for the minimal scalar product follows immediately from Lemma 3.3.

We now show that $p^*_{eig}(G) < 0$. Note that trace $\tilde{M}B\tilde{M} =$ trace $MB = 0$. Thus the sum of the eigenvalues of $\tilde{B} = \tilde{M}B\tilde{M}$ is 0. Let $\widehat{\phi}$ be a permutation of $\{1, \ldots, n\}$ that attains the minimum value $\min_{\phi \text{ permutation}} \sum_{i=1}^{k} \lambda_{\phi(i)}(G)\lambda_i(\tilde{B})$. Then for any permutation ψ, we have

$$\sum_{i=1}^{k} \lambda_{\psi(i)}(G)\lambda_i(\tilde{B}) \geq \sum_{i=1}^{k} \lambda_{\widehat{\phi}(i)}(G)\lambda_i(\tilde{B}). \tag{3.4}$$

Now if $\mathcal{T}$ is the set of all permutations of $\{1, 2, \ldots, n\}$, then we have

$$\begin{aligned}\sum_{\psi\in\mathcal{T}} \left(\sum_{i=1}^{k} \lambda_{\psi(i)}(G)\lambda_i(\tilde{B}) \right) &= \sum_{i=1}^{k} \left(\sum_{\psi\in\mathcal{T}} \lambda_{\psi(i)}(G) \right) \lambda_i(\tilde{B}) \\ &= \left(\sum_{\psi\in\mathcal{T}} \lambda_{\psi(1)}(G) \right) \left(\sum_{i=1}^{k} \lambda_i(\tilde{B}) \right) = 0, \end{aligned} \tag{3.5}$$

since $\sum_{\psi\in\mathcal{T}} \lambda_{\psi(i)}(G)$ is independent of i. This means that there exists at least one permutation ψ so that $\sum_{i=1}^{k} \lambda_{\psi(i)}(G)\lambda_i(\tilde{B}) \leq 0$, which implies that the minimal scalar product must satisfy $\sum_{i=1}^{k} \lambda_{\widehat{\phi}(i)}(G)\lambda_i(\tilde{B}) \leq 0$. Moreover, in view of (3.4) and (3.5), this minimal scalar product is zero if, and only if, $\sum_{i=1}^{k} \lambda_{\psi(i)}(G)\lambda_i(\tilde{B}) = 0$, for all $\psi \in \mathcal{T}$. Recall from Lemma 3.3 that $\lambda_1(\tilde{B}) > \lambda_k(\tilde{B})$. Moreover, if all eigenvalues of G were equal, then necessarily $G = \beta I$ for some $\beta \in \mathbb{R}$ and A must be diagonal. This implies that $A = 0$, a contradiction. This contradiction shows that $G(d)$ must have at least two distinct eigenvalues, regardless of the choice of d. Therefore, we can change the order and change the value of the scalar product on the left in (3.4). Thus $p^*_{eig}(G)$ is strictly negative.

Finally, the concavity follows by observing from (3.3) that

$$p^*_{eig}(G(d)) = \min_{Z^TZ=I} \frac{1}{2} \text{trace } G(d)Z(\tilde{M}B\tilde{M})Z^T$$

is a function obtained as a minimum of a set of functions affine in d, and recalling that the minimum of affine functions is concave. □

Remark 3.5 We emphasize here that the eigenvalue bounds depend on the choice of $d \in \mathbb{R}^n$. Though the d is irrelevant in Proposition 2.3, i.e., the function is equivalent on the feasible set of partition matrices $\mathcal{M}_m$, the values are no longer equal on the relaxed set $\mathcal{D}_O$. Of course the values are negative and not useful as a bound. We can fix $d = Ae \in \mathbb{R}^n$ and consider the bounds

$$\text{cut}(m) \geq 0 > p^*_{eig}(A - \gamma \,\text{Diag}(d)) = \frac{1}{2} \left\langle \lambda(A - \gamma \,\text{Diag}(d)), \begin{pmatrix} \lambda(\tilde{B}) \\ 0 \end{pmatrix} \right\rangle_{-}, \quad \gamma \geq 0.$$

From our empirical tests on random problems, we observed that the maximum occurs for γ closer to 0 than 1, thus illustrating why the bound using $G = A$ is better than the one using $G = -L$. This motivates our use of $G = A$ in the simulations below for the improved bounds.

3.2 Projected eigenvalue lower bounds

Projected eigenvalue bounds for the QAP, and for GP are presented and studied in [10,12,21]. They have proven to be surprisingly stronger than the basic eigenvalue bounds. (Seen to be < 0 above.) These are based on a special parametrization of the affine span of the linear equality constraints, $\mathcal{E}$. Rather than solving for the basic eigenvalue bound using the program in (3.1), we include the linear equality constraints $\mathcal{E}$, i.e., we consider the problem

$$\begin{array}{ll} \min & \frac{1}{2}\,\text{trace}\; GXBX^T \\ \text{s.t.} & X \in \mathcal{D}_O \cap \mathcal{E}, \end{array} \tag{3.6}$$

where $G = A - \text{Diag}(d)$, $d \in \mathbb{R}^n$.

We define the $n \times n$ and $k \times k$ orthogonal matrices P, Q with

$$P = \left[\tfrac{1}{\sqrt{n}}e \;\; V\right] \in \mathcal{O}_n, \quad Q = \left[\tfrac{1}{\sqrt{n}}\tilde{m} \;\; W\right] \in \mathcal{O}_k. \tag{3.7}$$

Lemma 3.6 [21, Lemma 3.1] *Let P, Q, V, W be defined in (3.7). Suppose that $X \in \mathbb{R}^{n\times k}$ and $Z \in \mathbb{R}^{(n-1)\times(k-1)}$ are related by*

$$X = P\begin{bmatrix} 1 & 0 \\ 0 & Z \end{bmatrix} Q^T\tilde{M}. \tag{3.8}$$

Then the following holds:

1. $X \in \mathcal{E}$.
2. $X \in \mathcal{N} \Leftrightarrow VZW^T \geq -\frac{1}{n}e\tilde{m}^T$.
3. $X \in \mathcal{D}_O \Leftrightarrow Z^TZ = I_{k-1}$.

Conversely, if $X \in \mathcal{E}$, then there exists Z such that the representation (3.8) holds. □

Let $\mathcal{Q} : \mathbb{R}^{(n-1)\times(k-1)} \to \mathbb{R}^{n\times k}$ be the linear transformation defined by $\mathcal{Q}(Z) = VZW^T\tilde{M}$ and define $\widehat{X} = \frac{1}{n}em^T \in \mathbb{R}^{n\times k}$. Then $\widehat{X} \in \mathcal{E}$, and Lemma 3.6 states that $\mathcal{Q}$ is an invertible transformation between $\mathbb{R}^{(n-1)\times(k-1)}$ and $\mathcal{E} - \widehat{X}$. Indeed, from (3.8), we see that $X \in \mathcal{E}$ if, and only if,

$$\begin{aligned} X &= P\begin{bmatrix} 1 & 0 \\ 0 & Z \end{bmatrix} Q^T\tilde{M} \\ &= \begin{bmatrix} \frac{e}{\sqrt{n}} & V \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & Z \end{bmatrix}\begin{bmatrix} \frac{1}{\sqrt{n}}\tilde{m}^T \\ W^T \end{bmatrix}\tilde{M} \\ &= \frac{1}{n}em^T + VZW^T\tilde{M} \\ &= \widehat{X} + VZW^T\tilde{M} = \widehat{X} + \mathcal{Q}(Z), \end{aligned} \tag{3.9}$$

for some Z. Thus, the set $\mathcal{E}$ can be parametrized using $\widehat{X} + VZW^T\tilde{M}$.

We are now ready to describe our two projected eigenvalue bounds. We remark that our bounds in (3.11) and in the first inequality in (3.14) were already discussed in [22, Proposition 3, Theorems 1, 3]. We include them for completeness. We note that the notation in Lemma 3.6, Eq. (3.9) and the next theorem will also be used frequently in Sect. 4 when we discuss the QP lower bound.

Theorem 3.7 *Let $d \in \mathbb{R}^n$, $G = A - \mathrm{Diag}(d)$. Let V, W be defined in (3.7) and $\widehat{X} = \frac{1}{n} em^T \in \mathbb{R}^{n\times k}$. Then:*

1. *For any $X \in \mathcal{E}$ and $Z \in \mathbb{R}^{(n-1)\times(k-1)}$ related by (3.9), we have*

$$\begin{aligned} \text{trace } GXBX^T &= \alpha + \text{trace } \widehat{G}Z\widehat{B}Z^T + \text{trace } CZ^T \\ &= -\alpha + \text{trace } \widehat{G}Z\widehat{B}Z^T + 2\,\text{trace } G\widehat{X}BX^T, \end{aligned} \tag{3.10}$$

and

$$\text{trace}(-L)XBX^T = \text{trace } \widehat{L}Z\widehat{B}Z^T, \tag{3.11}$$

where

$$\begin{aligned} &\widehat{G} = V^T GV, \widehat{L} = V^T(-L)V, \quad \widehat{B} = W^T\tilde{M}B\tilde{M}W, \\ &\alpha = \frac{1}{n^2}(e^T Ge)(m^T Bm), \quad C = 2V^T G\widehat{X}B\tilde{M}W. \end{aligned} \tag{3.12}$$

2. *We have the following two lower bounds:*
   (a)

$$\text{cut}(m) \geq p^*_{projeig}(G)$$

where

$$\begin{aligned} p^*_{projeig}(G) &:= \frac{1}{2}\left\{-\alpha + \left\langle \lambda(\widehat{G}), \begin{pmatrix}\lambda(\widehat{B}) \\ 0\end{pmatrix}\right\rangle_- + 2\min_{X\in\mathcal{D}} \text{trace } G\widehat{X}BX^T\right\} \\ &= \frac{1}{2}\left\{\alpha + \left\langle \lambda(\widehat{G}), \begin{pmatrix}\lambda(\widehat{B}) \\ 0\end{pmatrix}\right\rangle_- + \min_{0\leq\widehat{X}+VZW^T\tilde{M}} \text{trace } CZ^T\right\} \\ &= \frac{1}{2}\left\{-\alpha + \sum_{i=1}^{k-2}\lambda_{k-i}(\widehat{B})\lambda_i(\widehat{G}) + \lambda_1(\widehat{B})\lambda_{n-1}(\widehat{G})\right. \\ &\qquad \left. + 2\min_{X\in\mathcal{D}} \text{trace } G\widehat{X}BX^T\right\}. \end{aligned} \tag{3.13}$$

   (b)

$$\text{cut}(m) \geq p^*_{projeig}(-L) := \frac{1}{2}\left\langle \lambda(\widehat{L}), \begin{pmatrix}\lambda(\widehat{B}) \\ 0\end{pmatrix}\right\rangle_- \geq p^*_{eig}(-L). \tag{3.14}$$

Proof After substituting the parametrization (3.9) into the function trace $GXBX^T$, we obtain a constant, quadratic, and linear term:

$$\begin{aligned}\text{trace } GXBX^T &= \text{trace } G(\widehat{X} + VZW^T\tilde{M})B(\widehat{X} + VZW^T\tilde{M})^T \\ &= \text{trace } G\widehat{X}B\widehat{X}^T \\ &\quad + \text{trace}(V^TGV)Z(W^T\tilde{M}B\tilde{M}W)Z^T + \text{trace } 2V^TG\widehat{X}B\tilde{M}WZ^T\end{aligned}$$

and

$$\begin{aligned}\text{trace } GXBX^T &= \text{trace } G\widehat{X}B\widehat{X}^T + \text{trace}(V^TGV)Z(W^T\tilde{M}B\tilde{M}W)Z^T \\ &\quad + 2\,\text{trace } G\widehat{X}B(VZW^T\tilde{M})^T \\ &= \text{trace } G\widehat{X}B\widehat{X}^T + \text{trace}(V^TGV)Z(W^T\tilde{M}B\tilde{M}W)Z^T \\ &\quad + 2\,\text{trace } G\widehat{X}B(X - \widehat{X})^T \\ &= \text{trace}(-G)\widehat{X}B\widehat{X}^T + \text{trace}(V^TGV)Z(W^T\tilde{M}B\tilde{M}W)Z^T \\ &\quad + 2\,\text{trace } G\widehat{X}BX^T.\end{aligned}$$

These together with (3.12) yield the two equations in (3.10). Since $Le = 0$ and hence $L\widehat{X} = 0$, we obtain (3.11) on replacing G with $-L$ in the above relations. This proves Item 1.

We now prove (3.13), i.e., Item 2a. To this end, recall from (2.5) and (2.1) that

$$\text{cut}(m) = \min\left\{\frac{1}{2}\,\text{trace } GXBX^T : \; X \in \mathcal{D} \cap \mathcal{D}_O\right\}.$$

Combining this with (3.10), we see further that

$$\begin{aligned}\text{cut}(m) &= \frac{1}{2}\left(-\alpha + \min_{X\in\mathcal{D}\cap\mathcal{D}_O}\left\{\text{trace } \widehat{G}Z\widehat{B}Z^T + 2\,\text{trace } G\widehat{X}BX^T\right\}\right) \\ &\geq \frac{1}{2}\left(-\alpha + \min_{X\in\mathcal{E}\cap\mathcal{D}_O}\text{trace } \widehat{G}Z\widehat{B}Z^T + 2\min_{X\in\mathcal{D}}\text{trace } G\widehat{X}BX^T\right) \\ &= \frac{1}{2}\left(-\alpha + \left\langle\lambda(\widehat{G}), \begin{pmatrix}\lambda(\widehat{B}) \\ 0\end{pmatrix}\right\rangle_- + 2\min_{X\in\mathcal{D}}\text{trace } G\widehat{X}BX^T\right) \\ &= p^*_{projeig}(G), \end{aligned} \tag{3.15}$$

where Z and X are related via (3.9), and the last equality follows from Lemma 3.6 and Theorem 3.2. Furthermore, notice that

$$\begin{aligned}-\alpha + 2\min_{X\in\mathcal{D}}\text{trace } G\widehat{X}BX^T &= \alpha + 2\min_{X\in\mathcal{D}}\text{trace } G\widehat{X}B(X - \widehat{X})^T \\ &= \alpha + 2\min_{0\leq\widehat{X}+VZW^T\tilde{M}}\text{trace } G\widehat{X}B(VZW^T\tilde{M})^T \\ &= \alpha + \min_{0\leq\widehat{X}+VZW^T\tilde{M}}\text{trace } CZ^T, \end{aligned} \tag{3.16}$$

where the second equality follows from Lemma 3.6, and the last equality follows from the definition of C in (3.12). Combining this last relation with (3.15) proves the first two equalities in (3.13). The last equality in (3.13) follows from the fact that

$$\lambda_k(\tilde{B}) \le \lambda_{k-1}(\widehat{B}) \le \lambda_{k-1}(\tilde{B}) \le \cdots \le \lambda_2(\tilde{B}) = 0 \le \lambda_1(\widehat{B}) \le \lambda_1(\tilde{B}), \quad (3.17)$$

which is a consequence of the eigenvalue interlacing theorem [15, Corollary 4.3.16], the definition of $\widehat{B}$ and Lemma 3.3.

Next, we prove (3.14). Recall again from (2.5) and (2.1) that

$$\mathrm{cut}(m) = \min\left\{\frac{1}{2}\,\mathrm{trace}(-L)XBX^T : \ X \in \mathcal{D} \cap \mathcal{D}_O\right\}.$$

Using (3.11), we see further that

$$\begin{aligned}
\mathrm{cut}(m) &\ge \frac{1}{2}\min\left\{\mathrm{trace}(-L)XBX^T : \ X \in \mathcal{E} \cap \mathcal{D}_O\right\} \\
&= \frac{1}{2}\min\left\{\mathrm{trace}\,\widehat{L}Z\widehat{B}Z^T : \ X \in \mathcal{E} \cap \mathcal{D}_O\right\} \\
&= \frac{1}{2}\left\langle \lambda(\widehat{L}), \begin{pmatrix}\lambda(\widehat{B})\\ 0\end{pmatrix}\right\rangle_{-} \ (= p^*_{projeig}(-L)) \\
&\ge \min\left\{\frac{1}{2}\,\mathrm{trace}(-L)XBX^T : \ X \in \mathcal{D}_O\right\},
\end{aligned}$$

where Z and X are related via (3.9). The last inequality follows since the constraint $X \in \mathcal{E}$ is dropped. □

Remark 3.8 Let $Q \in \mathbb{R}^{(k-1)\times(k-1)}$ be the orthogonal matrix with columns consisting of the eigenvectors of $\widehat{B}$, defined in (3.12), corresponding to eigenvalues of $\widehat{B}$ in nondecreasing order; let $P_G, P_L \in \mathbb{R}^{(n-1)\times(k-1)}$ be the matrices with orthonormal columns consisting of $k-1$ eigenvectors of $\widehat{G}, \widehat{L}$, respectively, corresponding to the largest $k-2$ in nonincreasing order followed by the smallest. From (3.17) and Theorem 3.2, the minimal scalar product terms in (3.13) and (3.14), respectively, are attained at

$$Z_G = P_G Q^T, \quad Z_L = P_L Q^T, \quad (3.18)$$

respectively, and two corresponding points in $\mathcal{E}$ are given, according to (3.9), respectively, by

$$X_G = \widehat{X} + V Z_G W^T \tilde{M}, \quad X_L = \widehat{X} + V Z_L W^T \tilde{M}. \quad (3.19)$$

The linear programming problem, LP, in (3.13) can be solved explicitly; see Lemma 3.10 below. Since the condition number for the symmetric eigenvalue problem is 1, e.g., [9], the above shows that we can find the projected eigenvalue bounds very accurately. In addition, we need only find $k-1$ eigenvalues of $\widehat{G}$, $\widehat{B}$. Hence, if the

number of sets k is small relative to the number of nodes n and the adjacency matrix A is sparse, then we can find bounds for large problems both efficiently and accurately; see Sect. 7.2.

Remark 3.9 We emphasize again that although the objective function in (2.5) is equivalent for all $d \in \mathbb{R}^n$ on the set of partition matrices $\mathcal{M}_m$, this is not true once we relax this feasible set. Though there are advantages to using the Laplacian matrix as shown in [22] in terms of simplicity of the objective function, our numerics suggest that the bound $p^*_{projeig}(A)$ obtained from using the adjacency matrix A is stronger than $p^*_{projeig}(-L)$. Numerical tests confirming this are given in Sect. 7.

The constant term α and eigenvalue minimal scalar product term of the bound $p^*_{projeig}(G)$ in (3.13) can be found efficiently using the two quadratic forms for $\widehat{G}$, $\widehat{B}$ and finding $k-1$ eigenvalues from them. Before ending this section, we give an explicit solution to the linear optimization problem in (3.13) in Lemma 3.10, below, which constitutes the third term of the bound $p^*_{projeig}(G)$.

Notice that in (3.13), the minimization is taken over $X \in \mathcal{D}$, which is shown to be the convex hull of the set of partition matrices $\mathcal{M}_m$. As mentioned above, this essentially follows from the Birkhoff and Von Neumann theorems, see e.g., [23]. Thus, to solve the linear programming problem in (3.13), it suffices to consider minimizing the same objective over the nonconvex set $\mathcal{M}_m$ instead. This minimization problem has a closed form solution, as shown in the next Lemma. The simple proof follows by noting that every partition matrix can be obtained by permuting the rows of a specific partition matrix.

Lemma 3.10 *Let $d \in \mathbb{R}^n$, $G = A - \mathrm{Diag}(d)$, $\widehat{X} = \frac{1}{n} e m^T \in \mathcal{M}_m$ and*

$$v_0 = \begin{bmatrix} (n - m_k - m_1)e_{m_1} \\ (n - m_k - m_2)e_{m_2} \\ \vdots \\ (n - m_k - m_{k-1})e_{m_{k-1}} \\ 0e_{m_k} \end{bmatrix},$$

where $e_j \in \mathbb{R}^j$ is the vector of ones of dimension j. Then

$$\min_{X \in \mathcal{M}_m} \text{trace } G\widehat{X}BX^T = \frac{1}{n}\langle Ge, v_0\rangle_-.$$

4 Quadratic programming lower bound

A new successful and efficient bound used for the QAP is given in [1,5]. In this section, we adapt the idea described there to obtain a lower bound for cut(m). This bound uses a relaxation that is a *convex* QP, i.e., the minimization of a quadratic function that is convex on the feasible set defined by linear inequality constraints. Approaches based on nonconvex QPs are given in e.g., [13] and the references therein.

The main idea in [1,5] is to use the zero duality gap result for a homogeneous QAP [2, Theorem 3.2] on an objective obtained via a suitable reparametrization of the original problem. Following this idea, we consider the parametrization in (3.10) where our main objective in (2.5) is rewritten as:

$$\frac{1}{2}\,\text{trace}\; GXBX^T = \frac{1}{2}\left(\alpha + \text{trace}\,\widehat{G}Z\widehat{B}Z^T + \text{trace}\; CZ^T\right) \tag{4.1}$$

with X and Z related according to (3.8), and $G = A - \text{Diag}(d)$ for some $d \in \mathbb{R}^n$. We next look at the homogeneous part:

$$\begin{array}{rl} v_r^* := \min & \frac{1}{2}\,\text{trace}\,\widehat{G}Z\widehat{B}Z^T \\ \text{s.t.} & Z^TZ = I. \end{array} \tag{4.2}$$

Notice that the constraint $ZZ^T \preceq I$ is redundant for the above problem. By adding this redundant constraint, the corresponding Lagrange dual problem is given by

$$\begin{array}{rl} v_{dsdp} := \max & \frac{1}{2}\,\text{trace}\; S + \frac{1}{2}\,\text{trace}\; T \\ \text{s.t.} & I_{k-1} \otimes S + T \otimes I_{n-1} \preceq \widehat{B} \otimes \widehat{G}, \\ & S \preceq 0, \\ & S \in \mathcal{S}^{n-1},\; T \in \mathcal{S}^{k-1}, \end{array} \tag{4.3}$$

where the variables S and T are the dual variables corresponding to the constraints $ZZ^T \preceq I$ and $Z^TZ = I$, respectively. It is known that $v_r^* = v_{dsdp}$; see [19, Theorem 2]. This latter problem (4.3) can be solved efficiently. For example, as in the proofs of [2, Theorem 3.2] and [19, Theorem 2], one can take advantage of the properties of the Kronecker product and orthogonal diagonalizations of $\widehat{B}$, $\widehat{G}$, to reduce the problem to solving the following LP with $n + k - 2$ variables,

$$\begin{array}{rl} \max & \frac{1}{2}e^Ts + \frac{1}{2}e^Tt \\ \text{s.t.} & t_i + s_j \le \lambda_i\sigma_j, \quad i = 1,\ldots,k-1, \quad j = 1,\ldots,n-1, \\ & s_j \le 0, \quad j = 1,\ldots,n-1, \end{array} \tag{4.4}$$

where

$$\widehat{B} = U_1\,\text{Diag}(\lambda)U_1^T \;\text{ and }\; \widehat{G} = U_2\,\text{Diag}(\sigma)U_2^T \tag{4.5}$$

are eigenvalue orthogonal decompositions of $\widehat{B}$ and $\widehat{G}$, respectively. From an optimal solution (s^*, t^*) of (4.4), we can recover an optimal solution of (4.3) as

$$S^* = U_2\,\text{Diag}(s^*)U_2^T \qquad T^* = U_1\,\text{Diag}(t^*)U_1^T. \tag{4.6}$$

Next, suppose that the optimal value of the dual problem (4.3) is attained at (S^*, T^*). Let Z be such that the X defined according to (3.8) is a partition matrix. Then we have

$$\begin{aligned}\frac{1}{2}\operatorname{trace}(\widehat{G}Z\widehat{B}Z^T) &= \frac{1}{2}\operatorname{vec}(Z)^T(\widehat{B}\otimes\widehat{G})\operatorname{vec}(Z)\\ &= \frac{1}{2}\operatorname{vec}(Z)^T\underbrace{(\widehat{B}\otimes\widehat{G}-I\otimes S^*-T^*\otimes I)}_{\widehat{Q}}\operatorname{vec}(Z)\\ &\quad+\frac{1}{2}\operatorname{trace}(ZZ^TS^*)+\frac{1}{2}\operatorname{trace}(T^*)\\ &= \frac{1}{2}\operatorname{vec}(Z)^T\widehat{Q}\operatorname{vec}(Z)+\frac{1}{2}\operatorname{trace}([ZZ^T-I]S^*)+\frac{1}{2}\operatorname{trace}(S^*)\\ &\quad+\frac{1}{2}\operatorname{trace}(T^*)\\ &\geq \frac{1}{2}\operatorname{vec}(Z)^T\widehat{Q}\operatorname{vec}(Z)+\frac{1}{2}\operatorname{trace}(S^*)+\frac{1}{2}\operatorname{trace}(T^*),\end{aligned}$$

where the last inequality uses $S^* \preceq 0$ and $ZZ^T \preceq I$.

Recall that the original nonconvex problem (2.5) is equivalent to minimizing the right hand side of (4.1) over the set of all Z so that the X defined in (3.8) corresponds to a partition matrix. From the above relations, the third equality in (2.1) and Lemma 3.6, we see that

$$\begin{aligned}\operatorname{cut}(m) \geq \min\ & \tfrac{1}{2}(\alpha+\operatorname{trace}\ CZ^T+\operatorname{vec}(Z)^T\widehat{Q}\operatorname{vec}(Z))+\tfrac{1}{2}\operatorname{trace}(S^*)+\tfrac{1}{2}\operatorname{trace}(T^*)\\ \text{s.t.}\quad & Z^TZ=I_{k-1},\quad VZW^T\tilde{M}\geq-\widehat{X}.\end{aligned}\tag{4.7}$$

We also recall from (4.3) that $\frac{1}{2}\operatorname{trace}(S^*)+\frac{1}{2}\operatorname{trace}(T^*)=v_{dsdp}=v_r^*$, which further equals

$$\frac{1}{2}\left\langle\lambda(\widehat{G}),\begin{pmatrix}\lambda(\widehat{B})\\0\end{pmatrix}\right\rangle_-$$

according to (4.2) and Theorem 3.2.

A lower bound can now be obtained by relaxing the constraints in (4.7). For example, by dropping the orthogonality constraints, we obtain the following lower bound on $\operatorname{cut}(m)$:

$$\begin{aligned}p_{QP}^*(G) := \min\quad & q_1(Z)\\ \text{s.t.}\quad & VZW^T\tilde{M}\geq-\widehat{X},\end{aligned}$$

where

$$q_1(Z) := \frac{1}{2}\left(\alpha+\operatorname{trace}\ CZ^T+\operatorname{vec}(Z)^T\widehat{Q}\operatorname{vec}(Z)+\left\langle\lambda(\widehat{G}),\begin{pmatrix}\lambda(\widehat{B})\\0\end{pmatrix}\right\rangle_-\right).\tag{4.8}$$

Notice that this is a QP with $(n-1)(k-1)$ variables and nk constraints.

As in [1, p. 346], we now reformulate (4.8) into a QP in variables $X \in \mathcal{D}$, see (4.9). Note that the corresponding Hessian $\tilde{Q}$ defined in (4.10) is not positive semidefinite in general. Nevertheless, the QP is a convex problem.

Theorem 4.1 *Let S^*, T^* be optimal solutions of (4.3) as defined in (4.6). A lower bound on* cut(m) *is obtained from the following QP:*

$$\text{cut}(m) \geq p^*_{QP}(G) = \min_{X \in \mathcal{D}} \frac{1}{2} \text{vec}(X)^T \tilde{Q} \, \text{vec}(X) + \frac{1}{2} \left\langle \lambda(\widehat{G}), \begin{pmatrix} \lambda(\widehat{B}) \\ 0 \end{pmatrix} \right\rangle_{-}, \quad (4.9)$$

where

$$\tilde{Q} := B \otimes G - M^{-1} \otimes V S^* V^T - \tilde{M}^{-1} W T^* W^T \tilde{M}^{-1} \otimes I_n. \quad (4.10)$$

The QP in (4.9) is a convex problem since $\tilde{Q}$ is positive semidefinite on the tangent space of $\mathcal{E}$.

Proof We start by rewriting the second-order term of q_1 in (4.8) using the relation (3.8). Since $V^T V = I_{n-1}$ and $W^T W = I_{k-1}$, we have from the definitions of $\widehat{B}$ and $\widehat{G}$ that

$$\begin{aligned} \widehat{Q} &= \widehat{B} \otimes \widehat{G} - I_{k-1} \otimes S^* - T^* \otimes I_{n-1} \\ &= W^T \tilde{M} B \tilde{M} W \otimes V^T G V - I_{k-1} \otimes S^* - T^* \otimes I_{n-1} \\ &= (\tilde{M} W \otimes V)^T [B \otimes G - M^{-1} \otimes V S^* V^T \\ &\quad - \tilde{M}^{-1} W T^* W^T \tilde{M}^{-1} \otimes I_n] (\tilde{M} W \otimes V). \end{aligned} \quad (4.11)$$

On the other hand, from (3.9), we have

$$\text{vec}(X - \widehat{X}) = \text{vec}(V Z W^T \tilde{M}) = (\tilde{M} W \otimes V) \, \text{vec}(Z).$$

Hence, the second-order term in q_1 can be rewritten as

$$\text{vec}(Z)^T \widehat{Q} \, \text{vec}(Z) = \text{vec}(X - \widehat{X})^T \tilde{Q} \, \text{vec}(X - \widehat{X}), \quad (4.12)$$

where $\tilde{Q}$ is defined in (4.10). Next, we see from $V^T e = 0$ that

$$(M^{-1} \otimes V S^* V^T) \, \text{vec}(\widehat{X}) = \frac{1}{n} (M^{-1} \otimes V S^* V^T)(m \otimes I_n) e = \frac{1}{n} (e \otimes V S^* V^T) e = 0.$$

Similarly, since $W^T \tilde{m} = 0$, we also have

$$\begin{aligned} (\tilde{M}^{-1} W T^* W^T \tilde{M}^{-1} \otimes I_n) \, \text{vec}(\widehat{X}) &= \frac{1}{n} (\tilde{M}^{-1} W T^* W^T \tilde{M}^{-1} \otimes I_n)(m \otimes I_n) e \\ &= \frac{1}{n} (\tilde{M}^{-1} W T^* W^T \tilde{m} \otimes I_n) e = 0. \end{aligned}$$

Combining the above two relations with (4.12), we obtain further that

$$\begin{aligned}\operatorname{vec}(Z)^T \widehat{Q} \operatorname{vec}(Z) &= \operatorname{vec}(X)^T \tilde{Q} \operatorname{vec}(X) - 2 \operatorname{vec}(\widehat{X})^T [B \otimes G] \operatorname{vec}(X) \\ &\quad + \operatorname{vec}(\widehat{X})[B \otimes G] \operatorname{vec}(\widehat{X}) \\ &= \operatorname{vec}(X)^T \tilde{Q} \operatorname{vec}(X) - 2 \operatorname{trace}\, G \widehat{X} B X^T + \alpha.\end{aligned}$$

For the first two terms of q_1, proceeding as in (3.16), we have

$$\alpha + \operatorname{trace}\, C Z^T = -\alpha + 2 \operatorname{trace}\, G \widehat{X} B X^T.$$

Furthermore, recall from Lemma 3.6 that with X and Z related by (3.8), $X \in \mathcal{D}$ if, and only if, $V Z W^T \tilde{M} \geq -\widehat{X}$.

The conclusion in (4.9) now follows by substituting the above expressions into (4.8).

Finally, from (4.11) we see that $\tilde{Q}$ is positive semidefinite when restricted to the range of $\tilde{M} W \otimes V$. This is precisely the tangent space of $\mathcal{E}$. □

Although the dimension of the feasible set in (4.9) is slightly larger than the dimension of the feasible set in (4.8), the former feasible set is much simpler. Moreover, as mentioned above, even though $\tilde{Q}$ is not positive semidefinite in general, it is when restricted to the tangent space of $\mathcal{E}$. Thus, as in [5], one may apply the Frank–Wolfe algorithm on (4.9) to approximately compute the QP lower bound $p^*_{QP}(G)$ for problems with huge dimension.

Since $\widehat{Q} \succeq 0$, it is easy to see from (4.8) that $p^*_{QP}(G) \geq p^*_{projeig}(G)$. This inequality is not necessarily strict. Indeed, if $G = -L$, then $C = 0$ and $\alpha = 0$ in (4.8). Since the feasible set of (4.8) contains the origin, it follows from this and the definition of $p^*_{projeig}(-L)$ that $p^*_{QP}(-L) = p^*_{projeig}(-L)$. Despite this, as we see in the numerics Sect. 7, we have $p^*_{QP}(A) > p^*_{projeig}(A)$ for most of our numerical experiments. In general, we still do not know what conditions will guarantee $p^*_{QP}(G) > p^*_{projeig}(G)$.

5 Semidefinite programming lower bounds

In this section, we study the SDP relaxation constructed from the various equality constraints in the representation in (2.1) and the objective function in (2.4).

One way to derive an SDP relaxation for (2.5) is to start by considering a suitable Lagrangian relaxation, which is itself an SDP. Taking the dual of this Lagrangian relaxation then gives an SDP relaxation for (2.5); see [28,29] for the development for the QAP and GP cases, respectively. Alternatively, we can also obtain the *same* SDP relaxation directly using the well-known *lifting process*, e.g., [3,17,24,28,29]. In this approach, we start with the following equivalent quadratically constrained quadratic problems to (2.5):

$$\begin{array}{rll} \text{cut}(m) = \min & \frac{1}{2}\,\text{trace}\; GXBX^T = & \min \; \frac{1}{2}\,\text{trace}\; GXBX^T \\ \text{s.t.} & X \circ X = X, & \text{s.t.} \;\; X \circ X = x_0 X, \\ & \|Xe - e\|^2 = 0, & \quad\;\; \|Xe - x_0 e\|^2 = 0, \\ & \|X^T e - m\|^2 = 0, & \quad\;\; \|X^T e - x_0 m\|^2 = 0, \\ & X_{:i} \circ X_{:j} = 0, \;\; \forall i \neq j, & \quad\;\; X_{:i} \circ X_{:j} = 0, \;\; \forall i \neq j, \\ & X^T X - M = 0, & \quad\;\; X^T X - M = 0, \\ & \text{diag}(XX^T) - e = 0. & \quad\;\; \text{diag}(XX^T) - e = 0, \\ & & \quad\;\; x_0^2 = 1. \end{array} \tag{5.1}$$

Here: $G = A - \text{Diag}(d)$, $d \in \mathbb{R}^n$; the first equality follows from the fifth equality in (2.1), and we add x_0 and the constraint $x_0^2 = 1$ to *homogenize* the problem. Note that if $x_0 = -1$ at the optimum, then we can replace it with $x_0 = 1$ by changing the sign $X \leftarrow -X$ while leaving the objective value unchanged. We next linearize the quadratic terms in (5.1) using the matrix

$$Y_X := \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1 \;\; \text{vec}(X)^T).$$

Then $Y_X \succeq 0$ and is rank one. The objective function becomes

$$\frac{1}{2}\,\text{trace}\; GXBX^T = \frac{1}{2}\,\text{trace}\; L_G Y_X,$$

where

$$L_G := \begin{bmatrix} 0 & 0 \\ 0 & B \otimes G \end{bmatrix}. \tag{5.2}$$

By removing the rank one restriction on Y_X and using a general symmetric matrix variable Y rather than Y_X, we obtain the following SDP relaxation:

$$\begin{array}{rl} \text{cut}(m) \geq p^*_{SDP}(G) := \min & \frac{1}{2}\,\text{trace}\; L_G Y \\ \text{s.t.} & \text{arrow}\,(Y) = e_0, \\ & \text{trace}\; D_1 Y = 0, \\ & \text{trace}\; D_2 Y = 0, \\ & \mathcal{G}_J(Y) = 0, \\ & \mathcal{D}_O(Y) = M, \\ & \mathcal{D}_e(Y) = e, \\ & Y_{00} = 1, \\ & Y \succeq 0, \end{array} \tag{5.3}$$

where the rows and columns of $Y \in \mathcal{S}^{kn+1}$ are indexed from 0 to kn, and e_0 is the first (0th) unit vector. The notation used for describing the constraints above is standard; see, for example, [28]. For the convenience of the readers, we also describe them in detail in the "Appendix".

From the details in the "Appendix", we have that both D_1 and D_2 are positive semidefinite. From the constraints trace $D_i Y = 0, i = 1, 2$ we conclude that the feasible set of (5.3) has no strictly feasible (positive definite) point $Y \succ 0$. Numerical difficulties can arise when an interior-point method is directly applied to a problem where strict feasibility, Slater's condition, fails. Nonetheless, as in [28], we can find a simple matrix in the relative interior of the feasible set and use its structure to project (and regularize) the problem into a smaller dimension. This is achieved by finding a matrix V with range equal to the intersection of the nullspaces of D_1 and D_2. This is called *facial reduction*, [4,7]. Let $V_j \in \mathbb{R}^{j\times(j-1)}$, $V_j^T e = 0$, e.g.,

$$V_j := \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ 0 & 1 & \dots & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & 1 \\ -1 & \dots & \dots & -1 & -1 \end{bmatrix}_{j\times(j-1)}.$$

and let

$$\widehat{V} := \begin{bmatrix} 1 & 0 \\ \frac{1}{n} m \otimes e_n & V_k \otimes V_n \end{bmatrix},$$

where e_n is the vector of ones of dimension n. Then the range of $\widehat{V}$ is equal to the range of (any) $\widehat{Y} \in \text{relint } F$, the relative interior of the minimal face, and we can facially reduce (5.3) using the substitution

$$Y = \widehat{V} Z \widehat{V}^T \in \mathcal{S}^{kn+1}, \quad Z \in \mathcal{S}^{(k-1)(n-1)+1}.$$

The facially reduced SDP is then given by

$$\begin{aligned} \text{cut}(m) \geq p^*_{SDP}(G) = \min\ & \tfrac{1}{2} \text{trace } \widehat{V}^T L_G \widehat{V} Z \\ \text{s.t. } & \text{arrow}(\widehat{V} Z \widehat{V}^T) = e_0 \\ & \mathcal{G}_{\bar{J}}(\widehat{V} Z \widehat{V}^T) = \mathcal{G}_{\bar{J}}(e_0 e_0^T) \\ & \mathcal{D}_O(\widehat{V} Z \widehat{V}^T) = M \\ & \mathcal{D}_e(\widehat{V} Z \widehat{V}^T) = e \\ & Z \succeq 0, \quad Z \in \mathcal{S}^{(k-1)(n-1)+1}, \end{aligned} \tag{5.4}$$

where we let $\bar{J} := J \cup (0, 0)$.

We now present our final SDP relaxation (SDP$_{final}$) in Theorem 5.1 below and discuss some of its properties. This relaxation is surprisingly simple/strong with many of

the constraints in (5.4) redundant. In particular, we show that the problem is independent of the choice of $d \in \mathbb{R}^n$ in constructing G. We also show that the two constraints using $\mathcal{D}_O, \mathcal{D}_e$ are redundant in the SDP relaxation (SDP$_{final}$). This answers affirmatively the question posed in [28] on whether these constraints were redundant in the SDP relaxation for the GP.

Theorem 5.1 *The facially reduced SDP* (5.4) *is equivalent to the single equality constrained problem*

$$\begin{aligned} \text{cut}(m) \geq p^*_{SDP}(G) = \min\ & \tfrac{1}{2}\,\text{trace}\left(\widehat{V}^T L_G \widehat{V}\right) Z \\ \text{s.t. } & \mathcal{G}_{\bar{J}}(\widehat{V} Z \widehat{V}^T) = \mathcal{G}_{\bar{J}}(e_0 e_0^T) \qquad (SDP_{final}) \\ & Z \succeq 0, \quad Z \in \mathcal{S}^{(k-1)(n-1)+1}. \end{aligned}$$

The dual program is

$$\begin{aligned} \max\ & \tfrac{1}{2} W_{00} \\ \text{s.t. } & \widehat{V}^T \mathcal{G}_{\bar{J}}(W) \widehat{V} \preceq \widehat{V}^T L_G \widehat{V}. \end{aligned} \tag{5.5}$$

Both primal and dual satisfy Slater's constraint qualification and the objective function is independent of the $d \in \mathbb{R}^n$ chosen to form G.

Proof It is shown in [28] that the second constraint in (5.4) along with $Z \succeq 0$ implies that the arrow constraint holds, i.e., the arrow constraint is redundant. It only remains to show that the last two equality constraints in (5.4) are redundant. First, the gangster constraint using the linear transformation $\mathcal{G}_{\bar{J}}$ implies that the blocks in $Y = \widehat{V} Z \widehat{V}^T$ satisfy $\text{diag}\, \bar{Y}_{(ij)} = 0$ for all $i \neq j$, where $\bar{Y}$ respects the block structure described in (9.3). Next, we note that $D_i \succeq 0$, $i = 1, 2$ and $Y \succeq 0$. Therefore, the Schur complement of Y_{00} implies that

$$Y \succeq Y_{0:kn,0} Y_{0:kn,0}^T.$$

Writing $v_1 := Y_{0:kn,0}$ and $X = \text{Mat}(Y_{1:kn,0})$, we see further that

$$0 = \text{trace}(D_i Y) \geq \text{trace}(D_i v_1 v_1^T) = \begin{cases} \|Xe - e\|^2 & \text{if } i = 1, \\ \|X^T e - m\|^2 & \text{if } i = 2. \end{cases}$$

This together with the arrow constraints show that $\text{trace}\, \bar{Y}_{(ii)} = \sum_{j=(i-1)n+1}^{ni} Y_{j0} = m_i$. Thus, $\mathcal{D}_O(\widehat{V} Z \widehat{V}^T) = M$ holds. Similarly, one can see from the above and the arrow constraint that $\mathcal{D}_e(\widehat{V} Z \widehat{V}^T) = e$ holds.

The conclusion about Slater's constraint qualification for (SDP$_{final}$) follows from [28, Theorem 4.1], which discussed the primal SDP relaxations of the GP. That relaxation has the same feasible set as (SDP$_{final}$). In fact, it is shown in [28] that

$$\hat{Z} = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)} (n\,\text{Diag}(\bar{m}_{k-1}) - \bar{m}_{k-1} \bar{m}_{k-1}^T) \otimes (n I_{n-1} - E_{n-1}) \end{array}\right] \in \mathcal{S}_+^{(k-1)(n-1)+1},$$

where $\bar{m}_{k-1}^T = (m_1, \ldots, m_{k-1})$ and E_{n-1} is the $n-1$ square matrix of ones, is a strictly feasible point for (SDP$_{final}$). The right-hand side of the dual (5.5) differs from the dual of the SDP relaxation of the GP. However, let

$$\hat{W} = \begin{bmatrix} \alpha & 0 \\ 0 & (E_k - I_k) \otimes I_n \end{bmatrix}.$$

From the proof of [28, Theorem 4.2] we see that $\mathcal{G}_{\bar{J}}(\hat{W}) = \hat{W}$ and

$$\begin{aligned} -\widehat{V}^T \mathcal{G}_{\bar{J}}(\hat{W})\widehat{V} &= \widehat{V}^T(-\hat{W})\widehat{V} \\ &= \begin{bmatrix} 1 & m^T \otimes e^T/n \\ 0 & V_k^T \otimes V_n^T \end{bmatrix} \begin{bmatrix} -\alpha & 0 \\ 0 & ((I_k - E_k) \otimes I_n \end{bmatrix} \begin{bmatrix} 1 & 0 \\ m \otimes e/n & V_k \otimes V_n \end{bmatrix} \\ &= \begin{bmatrix} -\alpha + m^T(I_k - E_k)m/n & (m^T(I_k - E_k)V_k) \otimes (e^T V_n)/n \\ (V_k^T(I_k - E_k)m) \otimes (V_n^T e)/n & (V_k^T(I_k - E_k)V_k) \otimes (V_n^T V_n) \end{bmatrix} \\ &= \begin{bmatrix} -\alpha + m^T(I_k - E_k)m/n & 0 \\ 0 & (I_{k-1} + E_{k-1}) \otimes (I_{n-1} + E_{n-1}) \end{bmatrix} \\ &\succ 0, \qquad \text{for sufficiently large } -\alpha. \end{aligned}$$

Therefore $\widehat{V}^T \mathcal{G}_{\bar{J}}(\beta\hat{W})\widehat{V} \prec \widehat{V}^T L_G \widehat{V}$ for sufficiently large $-\alpha, \beta$, i.e., Slater's constraint qualification holds for the dual (5.5).

Finally, we let $Y = \widehat{V} Z \widehat{V}^T$ with Z feasible for (SDP$_{final}$). Then Y satisfies the gangster constraints, i.e., diag $\bar{Y}_{(ij)} = 0$ for all $i \neq j$. On the other hand, if we restrict $D = \text{Diag}(d)$, then the objective matrix L_D has nonzero elements only in the same diagonal positions of the off-diagonal blocks from the application of the Kronecker product $B \otimes \text{Diag}(d)$. Thus, we must have trace $L_D Y = 0$. Consequently, for all $d \in \mathbb{R}^n$,

$$\text{trace}\left(\widehat{V}^T L_G \widehat{V}\right) Z = \text{trace}\, L_G \widehat{V} Z \widehat{V}^T = \text{trace}\; L_G Y = \text{trace}\, L_A Y = \text{trace}\, \widehat{V} L_A \widehat{V}^T Z.$$

□

We next present two useful properties for finding/recovering approximate partition matrix solutions X from a solution Y of (SDP$_{final}$).

Proposition 5.2 *Suppose that Y is feasible for (SDP$_{final}$). Let $v_1 = Y_{1:kn,0}$ and $\begin{pmatrix} v_0 & v_2^T \end{pmatrix}^T$ denote a unit eigenvector of Y corresponding to the largest eigenvalue. Then $X_1 := \text{Mat}(v_1) \in \mathcal{E} \cap \mathcal{N}$. Moreover, if $v_0 \neq 0$, then $X_2 := \text{Mat}(\frac{1}{v_0} v_2) \in \mathcal{E}$. Furthermore, if, $Y \succeq 0$, then $v_0 \neq 0$ and $X_2 \in \mathcal{N}$.*

Proof The fact that $X_1 \in \mathcal{E}$ was shown in the proof of Theorem 5.1. That $X_1 \in \mathcal{N}$ follows from the arrow constraint. We now prove the results for X_2. Suppose first that $v_0 \neq 0$. Then

$$Y \succeq \lambda_1(Y) \begin{pmatrix} v_0 \\ v_2 \end{pmatrix} \begin{pmatrix} v_0 \\ v_2 \end{pmatrix}^T.$$

Using this and the definitions of D_i and X_2, we see further that

$$0 = \operatorname{trace}(D_i Y) \geq \begin{cases} \lambda_1(Y) v_0^2 \|X_2 e - e\|^2, & \text{if } i = 1, \\ \lambda_1(Y) v_0^2 \|X_2^T e - m\|^2, & \text{if } i = 2. \end{cases} \tag{5.6}$$

Since $\lambda_1(Y) \neq 0$ and $v_0 \neq 0$, it follows that $X_2 \in \mathcal{E}$.

Finally, suppose that $Y \geq 0$. We claim that any eigenvector $\begin{pmatrix} v_0 & v_2^T \end{pmatrix}^T$ corresponding to the largest eigenvalue must satisfy:

1. $v_0 \neq 0$;
2. all entries have the same sign, i.e., $v_0 v_2 \geq 0$.

From these claims, it would follow immediately that $X_2 = \operatorname{Mat}(v_2/v_0) \in \mathcal{N}$.

To prove these claims, we note first from the classical Perron–Fröbenius theory, e.g., [6], that the vector $\begin{pmatrix} |v_0| & |v_2|^T \end{pmatrix}^T$ is also an eigenvector corresponding to the largest eigenvalue.[2] Letting $\chi := \operatorname{Mat}(v_2)$ and proceeding as in (5.6), we conclude that

$$\|\chi e - v_0 e\|^2 = 0 \ \text{ and } \ \||\chi| e - |v_0| e\|^2 = 0.$$

The second equality implies that $v_0 \neq 0$. If $v_0 > 0$, then for all $i = 1, \ldots, n$, we have

$$\sum_{j=1}^{k} \chi_{ij} = v_0 = \sum_{j=1}^{k} |\chi_{ij}|,$$

showing that $\chi_{ij} \geq 0$ for all i, j, i.e., $v_2 \geq 0$. If $v_0 < 0$, one can show similarly that $v_2 \leq 0$. Hence, we have also shown $v_0 v_2 \geq 0$. This completes the proof. □

6 Feasible solutions and upper bounds

In the above we have presented several approaches for finding lower bounds for $\operatorname{cut}(m)$. In addition, we have found matrices X that approximate the bound and satisfy some of the graph partitioning constraints. Specifically, we obtain two approximate solutions $X_A, X_L \in \mathcal{E}$ in (3.19), an approximate solution to (4.8) which can be transformed into an $n \times k$ matrix via (3.9), and the X_1, X_2 described in Proposition 5.2. We now use these to obtain feasible solutions (partition matrices) and thus obtain upper bounds.

We show below that we can find the closest feasible partition matrix X to a given approximate matrix $\bar{X}$ using linear programming, where $\bar{X}$ is found, for example, using the projected eigenvalue, QP or SDP lower bounds. Note that (6.1) is a *transportation problem* and therefore the optimal X in (6.1) can be found in strongly polynomial time ($O(n^2)$), see e.g., [25,26].

[2] Indeed, if Y is irreducible, the largest in magnitude eigenvalue is positive and a singleton and the corresponding eigenspace is the span of a positive vector. Hence the conclusion follows. For a reducible Y, due to symmetry of Y, it is similar via permutation to a block diagonal matrix whose blocks are irreducible matrices. Thus, we can apply the same argument to conclude similar results for the eigenspace corresponding to the largest magnitude eigenvalue.

Theorem 6.1 *Let $\bar{X} \in \mathcal{E}$ be given. Then the closest partition matrix X to $\bar{X}$ in Fröbenius norm can be found by using the simplex method to solve the linear program*

$$\begin{array}{ll} \min & -\operatorname{trace} \bar{X}^T X \\ \text{s.t.} & Xe = e, \\ & X^T e = m, \\ & X \geq 0. \end{array} \tag{6.1}$$

Proof Observe that for any partition matrix X, trace $X^T X = n$. Hence, we have

$$\min_{X \in \mathcal{M}_m} \|\bar{X} - X\|_F^2 = \operatorname{trace}(\bar{X}^T \bar{X}) + n + 2 \min_{X \in \mathcal{M}_m} \operatorname{trace} \left(-\bar{X}^T X\right).$$

The result now follows from this and the fact that $\mathcal{M}_m = \operatorname{ext}(\mathcal{D})$, as stated in (2.1). (This is similar to what is done in [29].) □

7 Numerical tests

In this section, we provide empirical comparisons for the lower and upper bounds presented above. All the numerical tests are performed in MATLAB version R2012a on a *single* node of the *COPS* cluster at University of Waterloo. It is an SGI XE340 system, with two 2.4 GHz quad-core Intel E5620 Xeon 64-bit CPUs and 48 GB RAM, equipped with SUSE Linux Enterprise server 11 SP1.

7.1 Random tests with various sizes

In this subsection, we compare the bounds on structured graphs. These are formed by first generating k disjoint cliques (of sizes $m_1, \ldots, m_k$, randomly chosen from $\{2, ..., \mathsf{imax} + 1\}$). We join the first $k - 1$ cliques to every node of the kth clique. We then add u_0 edges between the first $k - 1$ cliques, chosen uniformly at random from the complement graph. In our tests, we set $u_0 = \lfloor e_c p \rfloor$, where e_c is the number of edges in the complement graph and $0 \leq p < 1$. By construction, $u_0 \geq \operatorname{cut}(m)$.

First, we note the following about the eigenvalue bounds. The two Figs. 1 and 2 show the difference in the projected eigenvalue bounds from using $A - \gamma \operatorname{Diag}(d)$ for a random $d \in \mathbb{R}^n$ on two structured graphs. This is typical of what we saw in our tests, i.e., that the maximum bound is near $\gamma = 0$. We had similar results for the specific choice $d = Ae$. This empirically suggests that using A would yield a better projected eigenvalue lower bound. This phenomenon leads us to use A in subsequent tests below.

In Table 1, we consider small instances where $k = 4, 5$, $p = 20\,\%$ and $\mathsf{imax} = 10$. We consider the projected eigenvalue bounds with $G = -L$ (eig_{-L}) and $G = A$ (eig_A), the QP bound with $G = A$, the SDP bound and the doubly nonnegative programming

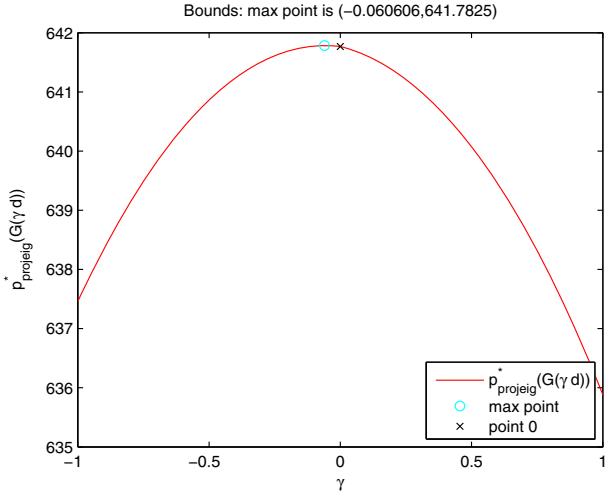

Fig. 1 Negative value for optimal γ

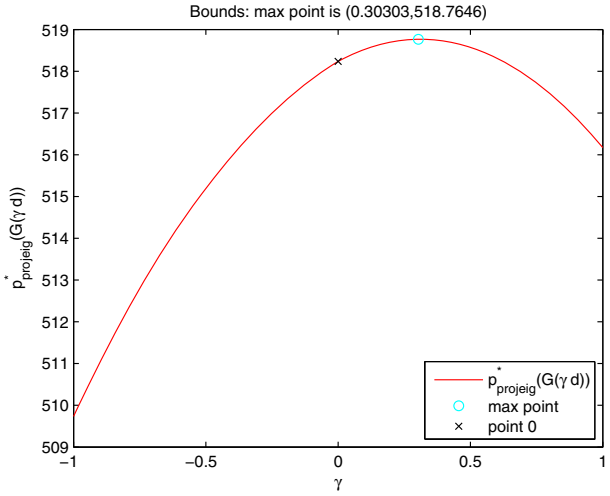

Fig. 2 Positive value for optimal γ

(DNN) bound.[3] For each approach, we present the lower bounds (rounded up to the nearest integer) and the corresponding upper bounds (rounded down to the nearest integer) obtained via the technique described in Sect. 6.[4] We also present the following

[3] The doubly nonnegative programming relaxation is obtained by imposing the constraint $\widehat{V}Z\widehat{V}^T \geq 0$ onto (SDP_{final}). Like the SDP relaxation, the bound obtained from this approach is independent of d. In our implementation, we picked $G = A$ for both the SDP and the DNN bounds.

[4] The SDP and DNN problems are solved via SDPT3 (version 4.0), [27], with tolerance gaptol set to be $1e{-}6$ and $1e{-}3$ respectively. The problems (4.4) and (4.8) are solved via SDPT3 (version 4.0) called by CVX (version 1.22), [11], using the default settings. The problem (6.1) is solved using simplex method in MATLAB, again using the default settings.

Table 1 Results for small structured graphs

Data				Lower bounds					Upper bounds					Gap
n	k	$\|E\|$	u_0	eig_{-L}	eig_A	QP	SDP	DNN	eig_{-L}	eig_A	QP	SDP	DNN	
31	4	362	25	21	22	24	23	25	68	102	25	36	25	0.0000
18	4	86	16	13	14	15	16	16	22	35	16	19	16	0.0000
29	5	229	44	32	37	40	39	44	76	74	44	53	44	0.0000
41	5	453	91	76	84	86	86	91	159	162	101	125	102	0.0521

Table 2 Results for medium-sized structured graphs

Data				Lower bounds				Upper bounds				Gap
n	k	$\|E\|$	u_0	eig_{-L}	eig_A	QP	SDP	eig_{-L}	eig_A	QP	SDP	
69	8	1077	317	249	283	290	281	516	635	328	438	0.0615
114	8	3104	834	723	785	794	758	1475	1813	834	1099	0.0246
85	8	2164	351	262	319	327	320	809	384	367	446	0.0576
116	10	3511	789	659	725	737	690	1269	2035	796	1135	0.0385
104	10	2934	605	500	546	554	529	1028	646	631	836	0.0650
78	10	1179	455	358	402	413	389	708	625	494	634	0.0893
129	12	3928	1082	879	988	1001	965	1994	1229	1233	1440	0.1022
120	12	3102	1009	833	913	926	893	1627	1278	1084	1379	0.0786
126	12	2654	1305	1049	1195	1218	1186	1767	1617	1361	1736	0.0554

measure of accuracy, defined as

$$\text{Gap} = \frac{\text{best upper bound} - \text{best lower bound}}{\text{best upper bound} + \text{best lower bound}}. \tag{7.1}$$

In terms of lower bounds, the DNN approach usually gives the best lower bounds. The SDP approach and the QP approach are comparable, while the projected eigenvalue lower bounds with A always outperforms the ones with $-L$. On the other hand, the DNN approach usually gives the best upper bounds.

We consider medium-sized instances in Table 2, where $k = 8, 10, 12$, $p = 20\,\%$ and $\mathsf{imax} = 20$. We do not consider DNN bounds due to computational complexity. We see that the lower bounds always satisfy $\text{eig}_{-L} \leq \text{eig}_A \leq \text{QP}$. In particular, we note that the (lower) projected eigenvalue bounds with A always outperform the ones with $-L$. However, what is surprising is that the lower projected eigenvalue bound with A sometimes outperforms the SDP lower bound. This illustrates the strength of the heuristic that replaces the quadratic objective function with the sum of a quadratic and linear term and then solves the linear part exactly over the partition matrices.

In Table 3, we consider larger instances with $k = 35, 45, 55$, $p = 20\,\%$ and $\mathsf{imax} = 100$. We do not consider SDP and DNN bounds due to computational complexity. We see again that the projected eigenvalue lower bounds with A always outperforms the ones with $-L$.

Table 3 Results for larger structured graphs

Data				Lower bounds		Upper bounds		Gap
n	k	$\|E\|$	u_0	eig_{-L}	eig_A	eig_{-L}	eig_A	
2012	35	575,078	361,996	345,251	356,064	442,567	377016	0.0286
1545	35	351,238	210,375	193,295	205,921	258,085	219,868	0.0328
1840	35	439,852	313,006	295,171	307,139	371,207	375,468	0.0944
1960	45	532,464	346,838	323,526	339,707	402,685	355,098	0.0222
2059	45	543,331	393,845	369,313	386,154	469,219	483,654	0.0971
2175	45	684,405	419,955	396,363	412,225	541,037	581,416	0.1351
2658	55	924,962	651,547	614,044	638,827	780,106	665,760	0.0206
2784	55	1,063,828	702,526	664,269	690,186	853,750	922,492	0.1059
2569	55	799,319	624,819	586,527	612,605	721,033	713,355	0.0760

We now briefly comment on the computational time (measured by MATLAB tic-toc function) for the above tests. For lower bounds, the eigenvalue bounds are fastest to compute. Computational time for small, medium and larger problems are usually less than 0.01 s, 0.1 s and 0.5 min, respectively. The QP bounds are more expensive to compute, taking around 0.5–2 s for small instances and 0.5 to 10 min for medium-sized instances. The SDP bounds are even more expensive to compute, taking 0.5–3 s for small instances and 2 min–2.5 h for medium-sized instances. The DNN bounds are the most expensive to compute. Even for small instances, it can take 20 s–40 min to compute a bound. For upper bounds, using the MATLAB simplex method, the time for solving (6.1) takes a few seconds for small and medium-sized problems; while for the larger problems in Tables 3, it takes 2–10 min.

Finding a vertex separator Before ending this subsection, we comment on how the above bounds can possibly be used in finding vertex separators when m is not explicitly known beforehand. Since there can be at most $\binom{n-1}{k-1}$ k-tuples of integers summing up to n, theoretically, one can consider all possible such m and estimate the corresponding $\text{cut}(m)$ with the bounds above.

As an illustration, we consider a concrete instance of a structured graph, generated with $n = 600$, $m_1 = m_2 = m_3 = 200$ and $p = 0$. Thus, we have $k = 3$, and, by construction, $\text{cut}(m) = 0$.

Suppose that the correct size vector m is not known in advance. Therefore we now consider a range of estimated vectors m'. In Table 4, we consider sizes m'_1 and m'_2 with values taken between 180 and 220, with $m'_3 = 600 - m'_1 - m'_2$. Since the roles of m'_1 and m'_2 are symmetric, we only include the cases where $m'_1 \le m'_2$. We report on the eigenvalue bounds, the QP bounds and the SDP bounds for each m'. Observe that the SDP lower bounds are usually the largest while the QP upper bounds are usually the smallest. The existence of a vertex separator when $m_1 = m_2 = m_3 = 200$ is identified by the QP and SDP bounds.[5] Furthermore, the QP upper bound being

[5] In this case, the approximate optimal value of (4.8) returned by the SDP solver is in the order of 10^{-5}. We obtain a 1 for the QP lower bound since we always round up to the smallest integer exceeding it.

Table 4 Results for medium-sized graph without an explicitly known m

Data		Lower bounds				Upper bounds			
m_1'	m_2'	eig_{-L}	eig_A	QP	SDP	eig_{-L}	eig_A	QP	SDP
180	180	−3600	−2400	−2400	−1800	2520	32,400	0	540
180	200	−1922	−1281	−1270	−949	2538	36,000	0	3240
180	220	−99	−66	−16	0	3600	39,600	3600	4312
200	200	0	0	1	0	2200	39,801	0	0
200	220	2074	2716	2759	4000	4000	40,000	4398	11, 832
220	220	4400	5867	5867	8400	8400	40,241	8400	12, 916

zero for the cases $(m_1', m_2') = (180, 180), (180, 200)$ also indicates the existence of a vertex separator.

7.2 Large sparse projected eigenvalue bounds

We assume that $n \gg k$. The projected eigenvalue bound in Theorem 3.7 in (3.13) is composed of a constant term, a minimal scalar product of $k-1$ eigenvalues and a linear term. The constant term and linear term are trivial to evaluate and essentially take no CPU time. The evaluation of the $k-1$ eigenvalues of $\widehat{B}$ is also efficient and accurate as the matrix is small and symmetric. The only significant cost is the evaluation of the largest $k-2$ eigenvalues and the smallest eigenvalue of $\widehat{G}$. In our test below, we use $G = A$ for simplicity. This choice is also justified by our numerical results in the previous subsection and the observation from Figs. 1 and 2.

We use the MATLAB *eigs* command for the $k-1$ eigenvalues of $V^T AV$ for the lower bound. Since the corresponding (6.1) has much larger dimension than we considered in the previous subsection, we turn to IBM ILOG CPLEX version 12.4 (MATLAB interface) with default settings to solve for the upper bound. We use the MATLAB tic-toc function to time the routine for finding the lower bound, and report output.time from the function cplexlp.m as the cputime for finding the upper bound.

We use two different choices V_0 and V_1 for the matrix V in (3.7).

1. We choose the following matrix V_0 with mutually orthogonal columns that satisfies $V_0^T e = 0$.[6]

$$V_0 = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ -1 & 1 & 1 & \dots & 1 \\ 0 & -2 & 1 & \dots & 1 \\ 0 & 0 & -3 & \dots & 1 \\ \dots & \dots & \dots & \dots & \\ 0 & 0 & 0 & \dots & -(n-1) \end{bmatrix}$$

[6] Choosing a sparse V in the orthogonal matrix in (3.7) would speed up the calculation of the eigenvalues. Choosing a sparse V would be easier if V did not require orthonormal columns but just linearly independent columns, i.e., if we could arrange for a parametrization as in Lemma 3.6 without P orthogonal.

Let $s = \left(\|V_0(:,i)\|\right) \in \mathbb{R}^{n-1}$. Then the operation needed for the MATLAB large sparse eigenvalue function *eigs* is ($*$ denotes multiplication and $\cdot'$ denotes transpose, ./ denotes elementwise division)

$$\widehat{A} * v = V' * (A * (V * v)) = V_0' * (A * (V_0 * (v./s)))./s. \tag{7.2}$$

Thus we never form the matrix $\widehat{A}$ and we preserve the structure of V_0 and sparsity of A when doing the matrix-vector multiplications.

2. An alternative approach uses

$$V_1 = \begin{bmatrix} \begin{bmatrix} \begin{bmatrix} I_{\lfloor \frac{n}{2} \rfloor} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{bmatrix} \\ 0_{(n-2\lfloor \frac{n}{2} \rfloor), \lfloor \frac{n}{2} \rfloor} \end{bmatrix} \begin{bmatrix} \begin{bmatrix} I_{\lfloor \frac{n}{4} \rfloor} \otimes \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix} \end{bmatrix} \\ 0_{(n-4\lfloor \frac{n}{4} \rfloor), \lfloor \frac{n}{4} \rfloor} \end{bmatrix} [\ldots] [\widehat{V}] \end{bmatrix}_{n \times n-1}$$

i.e., the block matrix consisting of t blocks formed from Kronecker products along with one block $\widehat{V}$ to complete the appropriate size so that $V^T V = I_{n-1}$, $V^T e = 0$. We take advantage of the 0, 1 structure of the Kronecker blocks and delay the scaling factors till the end. Thus we use the same type of operation as in (7.2) but with V_1 and the new scaling vector s.

The results on large scale problems using the two choices V_0 and V_1 are reported in Tables 5, 6 and 7. For simplicity, we only consider *random* graphs, with various imax and k and generate m as described in the beginning of Sect. 7.1. We then use the command

```
A=sprandsym(n,dens); A(1:n+1:end)=0; A(abs(A)>0)=1;
```

to generate a random incidence matrix, with dens $= 0.05/i$, for $i = 1, \ldots, 5$. In the tables, we present the number of nodes, sets, edges $(n, k, |E|)$, the true density of the random graph $density := 2|E|/(n(n-1))$, the lower and upper projected eigenvalue bounds, the gap (7.1), and the cputime (in seconds) for computing the bounds.

The results using the matrix V_0 are in Table 5. Here the cost for finding the lower bound using the eigenvalues becomes significantly higher than the cost for finding the upper bound using the simplex method.

Table 5 Large scale random graphs; imax 400; $k \in [65, 70]$, using V_0

n	k	$\|E\|$	Density	Lower	Upper	Gap	CPU (low)	CPU (up)
13,685	68	4,566,914	4.88×10^{-2}	3,958,917	4,271,928	0.0380	409.4	7.1
13,599	65	2,282,939	2.47×10^{-2}	1,967,979	2,181,778	0.0515	330.1	6.1
13,795	68	1,572,487	1.65×10^{-2}	1,314,033	1,495,421	0.0646	316.2	7.9
13,249	66	1,090,447	1.24×10^{-2}	832,027	985,375	0.0844	265.6	7.4
12,425	66	767,961	9.95×10^{-3}	589,226	710,093	0.0930	253.2	6.0

Table 6 Large scale random graphs; imax 400; $k \in [65, 70]$, using V_1

n	k	$\|E\|$	Density	Lower	Upper	Gap	CPU (low)	CPU (up)
14,680	69	5,254,939	4.88×10^{-2}	4,586,083	4,955,524	0.0387	262.9	6.4
14,464	65	2,583,109	2.47×10^{-2}	2,133,187	2,397,098	0.0583	135.5	6.0
14,974	69	1,852,955	1.65×10^{-2}	1,555,718	1,776,249	0.0662	98.2	6.9
13,769	65	1,177,579	1.24×10^{-2}	956,260	1,124,729	0.0810	44.4	5.9
13,852	69	954,632	9.95×10^{-3}	775,437	924,265	0.0876	51.3	6.0

Table 7 Large scale random graphs; imax 500; $k \in [75, 80]$, using V_1

n	k	$\|E\|$	Density	Lower	Upper	Gap	CPU (low)	CPU (up)
22,840	80	12,721,604	4.88×10^{-2}	11,548,587	12,262,688	0.0300	782.4	12.5
16,076	77	3,190,788	2.47×10^{-2}	2,754,650	3,053,622	0.0515	199.1	8.9
20,635	77	3,519,170	1.65×10^{-2}	2,916,188	3,287,657	0.0599	228.5	10.1
19,408	79	2,339,682	1.24×10^{-2}	1,989,278	2,272,340	0.0664	147.3	10.6
17,572	76	1,536,161	9.95×10^{-3}	1,188,933	1,417,085	0.0875	83.6	9.0

The results using the matrix V_1 are shown in Tables 6 and 7. We can see the obvious improvement in cputime when finding the lower bounds using V_1 compared to using V_0, which becomes more significant when the graph gets sparser.

In all three tables, we note that the relative gaps deteriorate as the density decreases. Also, the cputime for the eigenvalue bound is significantly better when using V_1 suggesting that sparsity of V_1 is better exploited in the MATLAB *eigs* command.

8 Conclusion

In this paper, we presented eigenvalue, projected eigenvalue, QP, and SDP lower and upper bounds for a minimum cut problem. In particular, we looked at a variant of the projected eigenvalue bound found in [22] and showed numerically that our variant is stronger. We also proposed a new QP bound following the approach in [1], making use of a duality result presented in [19]. In addition, we studied an SDP relaxation and demonstrated its strength by showing the redundancy of quadratic (orthogonality) constraints. We emphasize that these techniques for deriving bounds for our cut minimization problem can be adapted to derive new results for the GP. Specifically, one can easily adapt our derivation and obtain a QP lower bound for the GP, which was not previously known in the literature. Our derivation of the simple facially reduced SDP relaxation (SDP$_{final}$) can also be adapted to simplify the existing SDP relaxation for the GP studied in [28].

We also compared these bounds numerically on randomly generated graphs of various sizes. Our numerical tests illustrate that the projected eigenvalue bounds can

be found efficiently for large scale sparse problems and that they compare well against other more expensive bounds on smaller problems. It is surprising that the projected eigenvalue bounds using the adjacency matrix A are both cheap to calculate and strong.

Acknowledgments T. K. Pong was supported partly by a research grant from Hong Kong Polytechnic University. He was also supported as a PIMS postdoctoral fellow at Department of Computer Science, University of British Columbia, Vancouver, during the early stage of the preparation of the manuscript. Research of H. Sun supported by an Undergraduate Student Research Award from The Natural Sciences and Engineering Research Council of Canada. Research of N. Wang supported by The Natural Sciences and Engineering Research Council of Canada and by the U.S. Air Force Office of Scientific Research. H. Wolkowincz: Research supported in part by The Natural Sciences and Engineering Research Council of Canada and by the U.S. Air Force Office of Scientific Research.

Appendix: Notation for the SDP relaxation

In this appendix, we describes the constraints of the SDP relaxation (5.3) in detail.

1. The *arrow linear transformation* acts on $\mathcal{S}^{kn+1}$,

$$\operatorname{arrow}(Y) := \operatorname{diag}(Y) - (0, Y_{0,1:kn})^T, \tag{9.1}$$

   $Y_{0,1:kn}$ is the vector formed from the last kn components of the first row (indexed by 0) of Y. The arrow constraint represents $X \in \mathcal{Z}$.
2. The norm constraints for $X \in \mathcal{E}$ are represented by the constraints with the two $(kn+1) \times (kn+1)$ matrices

$$D_1 := \begin{bmatrix} n & -e_k^T \otimes e_n^T \\ -e_k \otimes e_n & (e_k e_k^T) \otimes I_n \end{bmatrix},$$
$$D_2 := \begin{bmatrix} m^T m & -m^T \otimes e_n^T \\ -m \otimes e_n & I_k \otimes (e_n e_n^T) \end{bmatrix},$$

   where e_j is the vector of ones of dimension j.
3. We let $\mathcal{G}_J$ represent the gangster operator on $\mathcal{S}^{kn+1}$, i.e., it shoots *holes/zeros* in a matrix,

$$(\mathcal{G}_J(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } (i,j) \text{ or } (j,i) \in J \\ 0 & \text{otherwise,} \end{cases}$$
$$J := \{(i,j) : i = (p-1)n + q, \quad j = (r-1)n + q, \quad \text{for } \begin{array}{l} p < r, \ p, r \in \{1, \ldots, k\} \\ q \in \{1, \ldots, n\} \end{array} \Big\}. \tag{9.2}$$

   The gangster constraint represents the (Hadamard) orthogonality of the columns of X. The positions of the zeros are the diagonal elements of the off-diagonal blocks $\bar{Y}_{(ij)}$, $1 < i < j$, of Y; see the block structure in (9.3) below.

4. Again, by abuse of notation, we use the symbols for the sets of constraints $\mathcal{D}_O$, $\mathcal{D}_e$ to represent the linear transformations in the SDP relaxation (5.3). Note that

$$\langle \Psi, X^T X \rangle = \text{trace } I X \Psi X^T = \text{vec}(X)^T (\Psi \otimes I) \,\text{vec}(X).$$

Therefore, the adjoint of $\mathcal{D}_O$ is made up of a zero row/column and k^2 blocks that are multiples of the identity:

$$\mathcal{D}_O^*(\Psi) = \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & \Psi \otimes I_n \end{array}\right].$$

If Y is blocked appropriately as

$$Y = \left[\begin{array}{c|c} Y_{00} & Y_{0,:} \\ \hline Y_{:,0} & \bar{Y} \end{array}\right], \quad \bar{Y} = \begin{bmatrix} \bar{Y}_{(11)} & \bar{Y}_{(12)} & \cdots & \bar{Y}_{(1k)} \\ \bar{Y}_{(21)} & \bar{Y}_{(22)} & \cdots & \bar{Y}_{(2k)} \\ \vdots & \ddots & \ddots & \vdots \\ \bar{Y}_{(k1)} & \ddots & \ddots & \bar{Y}_{(kk)} \end{bmatrix}, \tag{9.3}$$

with each $\bar{Y}_{(ij)}$ being a $n \times n$ matrix, then

$$\mathcal{D}_O(Y) = \left(\text{trace } \bar{Y}_{(ij)}\right) \in \mathcal{S}^k. \tag{9.4}$$

Similarly,

$$\langle \phi, \text{diag}(X X^T) \rangle = \langle \text{Diag}(\phi), X X^T \rangle = \text{vec}(X)^T \, (I_k \otimes \text{Diag}(\phi)) \,\text{vec}(X).$$

Therefore we get the sum of the diagonal parts

$$\mathcal{D}_e(Y) = \sum_{i=1}^{k} \text{diag } \bar{Y}_{(ii)} \in \mathbb{R}^n. \tag{9.5}$$

References

1. Anstreicher, K.M., Brixius, N.W.: A new bound for the quadratic assignment problem based on convex quadratic programming. Math. Program. **89**(3, Ser. A), 341–357 (2001)
2. Anstreicher, K.M., Wolkowicz, H.: On Lagrangian relaxation of quadratic matrix constraints. SIAM J. Matrix Anal. Appl. **22**(1), 41–55 (2000)
3. Balas, E., Ceria, S., Cornuejols, G.: A lift-and-project cutting plane algorithm for mixed 0–1 programs. Math. Program. **58**, 295–324 (1993)
4. Borwein, J.M., Wolkowicz, H.: Facial reduction for a cone-convex programming problem. J. Aust. Math. Soc. A **30**(3), 369–380 (1980/1981)
5. Brixius, N.W., Anstreicher, K.M.: Solving quadratic assignment problems using convex quadratic programming relaxations. Optim. Methods Softw. **16**(1–4), 49–68 (2001). Dedicated to Professor Laurence C. W. Dixon on the occasion of his 65th birthday
6. Brualdi, R.A., Ryser, H.J.: Combinatorial Matrix Theory. Cambridge University Press, New York (1991)

7. Cheung, Y.-L., Schurr, S., Wolkowicz, H.: Preprocessing and regularization for degenerate semidefinite programs. In: Bailey, D.H., Bauschke, H.H., Borwein, P., Garvan, F., Thera, M., Vanderwerff, J., Wolkowicz, H. (eds.) Computational andAnalytical Mathematics. In Honor of Jonathan Borwein's 60thBirthday. Springer Proceedings in Mathematics & Statistics, vol. 50, pp. 225–276. Springer, New York (2013)
8. de Klerk, E., Nagy, M.E., Sotirov, R.: On semidefinite programming bounds for graph bandwidth. Optim. Methods Softw. **28**(3), 485–500 (2013)
9. Demmel, J.W.: Applied Numerical Linear Algebra. Society for Industrial and Applied Mathematics (SIAM), Philadelphia (1997)
10. Falkner, J., Rendl, F., Wolkowicz, H.: A computational study of graph partitioning. Math. Program. **66**(2, Ser. A), 211–239 (1994)
11. Grant, M., Boyd, S., Ye, Y.: Disciplined convex programming. In: Global Optimization. Nonconvex Global Optimization, vol. 84, pp. 155–210. Springer, New York (2006)
12. Hadley, S.W., Rendl, F., Wolkowicz, H.: A new lower bound via projection for the quadratic assignment problem. Math. Oper. Res. **17**(3), 727–739 (1992)
13. Hager, W.W., Hungerford, J.T.: A continuous quadratic programming formulation of the vertex separator problem. Report, University of Florida, Gainesville (2013)
14. Hoffman, A.J., Wielandt, H.W.: The variation of the spectrum of a normal matrix. Duke Math. **20**, 37–39 (1953)
15. Horn, R.A., Johnson, C.R.: Matrix Analysis. Cambridge University Press, Cambridge (1990). Corrected reprint of the 1985 original
16. Lewis, R.H.: Yet another graph partitioning problem is NP-Hard. Report. arXiv:1403.5544 [cs.CC] (2014)
17. Lovász, L., Schrijver, A.: Cones of matrices and set-functions and 0–1 optimization. SIAM J. Optim. **1**(2), 166–190 (1991)
18. Martí, R., Campos, V., Piñana, E.: A branch and bound algorithm for the matrix bandwidth minimization. Eur. J. Oper. Res. **186**(2), 513–528 (2008)
19. Povh, J., Rendl, F.: Approximating non-convex quadratic programs by semidefinite and copositive programming. In: KOI 2006—11th International Conference on Operational Research, pp. 35–45. Croatian Operational Research Review, Zagreb (2008)
20. Rendl, F., Wolkowicz, H.: Applications of parametric programming and eigenvalue maximization to the quadratic assignment problem. Math. Program. **53**(1, Ser. A), 63–78 (1992)
21. Rendl, F., Wolkowicz, H.: A projection technique for partitioning the nodes of a graph. Ann. Oper. Res. **58**, 155–179 (1995). Applied mathematical programming and modeling, II (APMOD 93) (Budapest, 1993)
22. Rendl, F., Lisser, A., Piacentini, M.: Bandwidth, vertex separators and eigenvalue optimization. In: Discrete Geometry and Optimization. The Fields Institute for Research in Mathematical Sciences. Communications Series. pp. 249–263. Springer, New York (2013)
23. Schrijver, A.: Theory of Linear and Integer Programming. Wiley-Interscience Series in Discrete Mathematics. Wiley, Chichester (1986)
24. Sherali, H.D., Adams, W.P.: Computational advances using the reformulation-linearization technique (rlt) to solve discrete and continuous nonconvex problems. Optima **49**, 1–6 (1996)
25. Tardos, E.: A strongly polynomial algorithm to solve combinatorial linear programs. Oper. Res. **34**(2), 250–256 (1986)
26. Tardos, E.: Strongly polynomial and combinatorial algorithms in optimization. In: Proceedings of the International Congress of Mathematicians, Vol. I, II (Kyoto, 1990), pp. 1467–1478. Mathematical Society of Japan, Tokyo (1991)
27. Tütüncü, R.H., Toh, K.C., Todd, M.J.: Solving semidefinite-quadratic-linear programs using SDPT3. Math. Program. **95**(2, Ser. B), 189–217 (2003). Computational semidefinite and second order cone programming: the state of the art
28. Wolkowicz, H., Zhao, Q.: Semidefinite programming relaxations for the graph partitioning problem. Discrete Appl. Math. **96**(97), 461–479 (1999). Selected for the special Editors' Choice, Edition 1999
29. Zhao, Q., Karisch, S.E., Rendl, F., Wolkowicz, H.: Semidefinite programming relaxations for the quadratic assignment problem. J. Comb. Optim. **2**(1), 71–109 (1998). Semidefinite programming and interior-point approaches for combinatorial optimization problems (Fields Institute, Toronto, ON, 1996)