




Connectivity via convexity: Bounds on the edge expansion in graphs

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Convexification techniques have gained increasing interest over the past decades. In this work, we apply a recently developed convexification technique for fractional programs by He, Liu and Tawarmalani (2024) to the problem of determining the edge expansion of a graph. Computing the edge expansion of a graph is a well-known, difficult combinatorial problem that seeks to partition the graph into two sets such that a fractional objective function is minimized.

We give a formulation of the edge expansion as a completely positive program and propose a relaxation as a doubly non-negative program, further strengthened by cutting planes. Additionally, we develop an augmented Lagrangian algorithm to solve the doubly non-negative program, obtaining lower bounds on the edge expansion. Numerical results confirm that this relaxation yields strong bounds and is computationally efficient, even for graphs with several hundred vertices.

Keywords: edge expansion, Cheeger constant, completely positive program, doubly non-negative relaxation, augmented Lagrangian method

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1 Introduction

Let $G = (V, E)$ be a simple graph on $n \geq 3$ vertices. The edge expansion of G is defined as

$$h(G) = \min_{\emptyset \neq S \subset V} \frac{|\partial S|}{\min\{|S|, |V \setminus S|\}},$$

where $\partial S = \{\{i, j\} \in E : i \in S, j \notin S\}$ is the cut induced by the set S . This graph parameter is also known under the name *Cheeger constant* or *isoperimetric number* or *sparsest cut*.

This constant is positive if and only if the graph is connected. A graph with $h(G) \geq c$, for some constant $c > 0$, is called a c -expander. A graph with $h(G) < 1$ is said to have a bottleneck since there are not too many edges across it. The famous conjecture of Mihail-Vazirani [22, 10] in polyhedral combinatorics claims that the graph (1-skeleton) of any 0/1-polytope has edge expansion at least 1. This has been proven to be true for several combinatorial polytopes [22, 18] and bases-exchange graphs of matroids [1], and a weaker form was established recently for random 0/1-polytopes [20]. The edge expansion problem arises in several applications. For references and for relations to similar problems, we refer the reader to the recent paper [12].

The edge expansion problem belongs to the class of combinatorial fractional programming problems. Fractional programming has been studied at least since the sixties of the 20th century [9, 8]. It finds applications in fields like economics, engineering, and telecommunications. While there are fractional programs that can be solved in polynomial time [8], the edge expansion problem and many other fractional programs do not admit polynomial time algorithms. For more details on applications and on known results of fractional programming, we refer to the comprehensive literature review in [13].

In [12] two exact algorithms based on semidefinite programming to compute $h(G)$ have been developed. In the first algorithm, the problem is split into several k -bisection problems. Limiting the number of candidates to be considered for k as well as computing the k -bisection is done using strong bounds from semidefinite programming. The other algorithm in [12] uses an idea of Dinkelbach and computes the edge expansion by considering several parametrized optimization problems, which can all be solved using a max-cut solver.

We now take a different direction, and instead of transforming the problem into several instances of known combinatorial optimization problems, we want to obtain strong lower bounds on the edge expansion itself by using a doubly non-negative relaxation. This relaxation results from applying a convexification technique for fractional programs, developed recently by He, Liu and Tawarmalani [13].

The main contributions of this paper are as follows.

- We convexify the edge expansion problem and write it as a completely positive program.
- We relax this completely positive program to a doubly non-negative program and strengthen it with additional inequalities.

- We develop and implement an augmented Lagrangian algorithm tailored for the derived relaxation.
- The quality of the bounds produced by the relaxation and the effectiveness of our algorithm are illustrated by numerical results.
- All code and data sets are publicly available as open source.

Outline This paper is structured as follows. We next formulate the problem as a binary fractional optimization problem and derive a basic doubly non-negative relaxation. In Section 3.1 we state the main result of [13] that we apply in Section 3.2 to give a formulation of the edge expansion as a completely positive program. In Section 4, we then relax the completely positive program to a doubly non-negative programming problem, propose a facial reduction approach, and prove that the new bound is at least as good as the one from the basic relaxation. An augmented Lagrangian algorithm for solving the relaxation is presented in Section 5. Section 6 shows that, indeed, the relaxation is improving over the basic relaxation significantly and demonstrates the efficiency of the bounding routine. We conclude the paper in Section 7.

Notation The set of $n \times n$ real symmetric matrices is denoted by \mathcal{S}^n . The positive semidefiniteness condition for $X \in \mathcal{S}^n$ is written as $X \succeq 0$, and we denote by $\mathcal{P}_{\succeq 0}(X)$ the projection of X onto the cone of positive semidefinite matrices. We write $X \geq 0$ to denote that a matrix X is entry wise non-negative and $X \in \text{DNN}$ if $X \succeq 0$ and $X \geq 0$. The trace of X is written as $\text{tr}(X)$ and defined as the sum of its diagonal elements. The trace inner product for $X, Y \in \mathcal{S}^n$ is defined as $\langle X, Y \rangle = \text{tr}(XY)$, and we denote the Frobenius norm of X by $\|X\| = \sqrt{\langle X, X \rangle}$. The operator $\text{diag}(X)$ returns the main diagonal of matrix X as a vector. The operator $\text{Diag}: \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$ yields the diagonal matrix with its diagonal equal to the vector and $\text{Diag}(M_1, M_2, \dots, M_k)$ returns the block-diagonal matrix constructed by the input matrices and by the diagonal matrices formed from all the arguments, which are vectors. The symbol \otimes denotes the Kronecker product. The vector of all ones of size n is denoted by e_n , the vector of all zeros of size n is denoted by 0_n , and I_n is the $n \times n$ identity matrix. By E_n , we denote the matrix of all ones, and u_i is the standard unit vector with entry i equal to 1. All the subscripts are omitted if the size is clear from the context.

2 A basic DNN relaxation for edge expansion

The edge expansion problem can be formulated as the binary fractional optimization problem

$$\begin{aligned}
 h(G) = \min \quad & \frac{\bar{x}^\top L \bar{x}}{e^\top \bar{x}} \\
 \text{s.t.} \quad & 1 \leq e^\top \bar{x} \leq \left\lfloor \frac{n}{2} \right\rfloor \\
 & \bar{x} \in \{0, 1\}^n,
 \end{aligned} \tag{1}$$

where L denotes the Laplacian matrix of G that is defined as

$$L_{ij} = \begin{cases} -1, & \text{if } \{i, j\} \in E, \\ \text{deg}(i), & \text{if } i = j \text{ and} \\ 0, & \text{otherwise.} \end{cases}$$

To obtain a doubly non-negative relaxation (DNN) for (1), one can linearize the objective function by introducing a matrix variable, which results in a matrix lifting relaxation. Let $X = \bar{x}\bar{x}^\top$ and $\rho = \frac{1}{e^\top \bar{x}}$. Then the matrix $\bar{Y} = \rho X$ and the vector $\bar{y} = \rho \bar{x}$ satisfy the following conditions. First, we have

$$e^\top \bar{y} = e^\top (\rho \bar{x}) = \frac{e^\top \bar{x}}{e^\top \bar{x}} = 1.$$

Then, because of the constraints $1 \leq e^\top \bar{x} \leq \lfloor \frac{n}{2} \rfloor$, it follows that

$$\frac{1}{\lfloor \frac{n}{2} \rfloor} \leq \rho \leq 1.$$

From $\langle E, \bar{Y} \rangle = \text{tr}(ee^\top (\rho \bar{x}\bar{x}^\top)) = \frac{(e^\top \bar{x})^2}{e^\top \bar{x}} = e^\top \bar{x}$ we get

$$1 \leq \langle E, \bar{Y} \rangle \leq \lfloor \frac{n}{2} \rfloor.$$

For $\bar{x}_i \in \{0, 1\}$, we have $\bar{x}_i^2 = \bar{x}_i$ and hence,

$$\text{diag}(\bar{Y}) = \text{diag}(\rho \bar{x}\bar{x}^\top) = \rho \bar{x} = \bar{y}.$$

The non-convex constraint $X - \bar{x}\bar{x}^\top = 0$ is relaxed to $X - \bar{x}\bar{x}^\top \succeq 0$, which is equivalent to $\begin{pmatrix} X & \bar{x} \\ \bar{x}^\top & 1 \end{pmatrix} \succeq 0$ by the well-known Schur complement. Multiplying by $\rho > 0$ gives

$$\begin{pmatrix} \bar{Y} & \bar{y} \\ \bar{y}^\top & \rho \end{pmatrix} \succeq 0.$$

Furthermore, the objective function can be written as

$$\frac{\bar{x}^\top L \bar{x}}{e^\top \bar{x}} = \frac{\langle L, X \rangle}{e^\top \bar{x}} = \langle L, \rho X \rangle = \langle L, \bar{Y} \rangle.$$

After putting these constraints together and adding $\begin{pmatrix} \bar{Y} & \bar{y} \\ \bar{y}^\top & \rho \end{pmatrix} \geq 0$, we arrive at the following basic DNN relaxation for the edge expansion problem.

$$\begin{aligned}
\min \quad & \langle L, \bar{Y} \rangle \\
\text{s.t.} \quad & e^\top \bar{y} = 1 \\
& \frac{1}{\lfloor \frac{n}{2} \rfloor} \leq \rho \leq 1 \\
& 1 \leq \langle E, \bar{Y} \rangle \leq \lfloor \frac{n}{2} \rfloor \\
& \text{diag}(\bar{Y}) = \bar{y} \\
& \begin{pmatrix} \bar{Y} & \bar{y} \\ \bar{y}^\top & \rho \end{pmatrix} \in \text{DNN}.
\end{aligned} \tag{DNN}_{n+1}$$

We call this a basic DNN relaxation since it does not contain additional cutting planes such as triangle inequalities, etc. Adding a rank-constraint to (DNN_{n+1}) results in computing $h(G)$. We will later relate (DNN_{n+1}) to the relaxation which we are going to derive in the next section.

3 Convexification of the edge expansion

In this section, we apply the recent convexification results of He, Liu, and Tawarmalani in [13] to reformulate the edge expansion problem. For this, we start by presenting the main results needed from that paper.

3.1 A convexification technique for fractional programs

The first important result on the convexification for fractional programs is the following.

Theorem 1 (Theorem 2 of [13]). *Let $f: \mathcal{X} \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $f(x) = (f_1(x), \dots, f_m(x))^\top$ be a vector of base functions. And let another vector be obtained from the base functions by dividing each of them with a linear form of f . We then define the following two sets.*

$$\begin{aligned}
\mathcal{F} &= \{f(x) : x \in \mathcal{X}\} \\
\mathcal{G} &= \left\{ \frac{f(x)}{\sum_{i \in [m]} \alpha_i f_i(x)} : x \in \mathcal{X} \right\}
\end{aligned}$$

We assume that \mathcal{F} is bounded and there exists $\varepsilon > 0$ such that $\sum_{i \in [m]} \alpha_i f_i(x) > \varepsilon$ for all $x \in \mathcal{X}$. Then,

$$\text{conv}(\mathcal{G}) = \{g \in \mathbb{R}^m : g \in \rho \text{conv}(\mathcal{F}), \alpha^\top g = 1, \rho \geq 0\} \tag{2}$$

and if $f_1(x) = 1$, then

$$\text{conv}(\mathcal{F}) = \{f \in \mathbb{R}^m : f \in \sigma \text{conv}(\mathcal{G}), f_1 = 1, \sigma \geq 0\}. \tag{3}$$

This theorem is used to reformulate quadratic fractional binary optimization problems to optimization problems over the completely positive cone. Let $\mathcal{X} \subseteq \mathbb{R}^n$ and \mathcal{L} be an affine set of \mathbb{R}^n . We consider the following minimization problem

$$\min_{x \in \mathcal{X} \cap \mathcal{L}} \frac{x^\top Bx + b^\top x + b_0}{x^\top Ax + a^\top x + a_0} \quad (4)$$

and set $q(x) := x^\top Ax + a^\top x + a_0$ to be the denominator of the objective function. We assume that $\mathcal{X} \cap \mathcal{L}$ is non-empty, bounded and that for all elements $x \in \mathcal{X} \cap \mathcal{L}$ it holds $q(x) > 0$. Let further

$$\mathcal{G}' = \left\{ \frac{(1, x, xx^\top)}{q(x)} : x \in \mathcal{X} \cap \mathcal{L} \right\},$$

then (4) is equivalent to

$$\min \{ \langle B, Y \rangle + b^\top y + b_0 \rho : (\rho, y, Y) \in \mathcal{G}' \}. \quad (5)$$

One could equivalently also optimize the linear objective over the convex hull $\text{conv}(\mathcal{G}')$. To do so, the authors of [13] showed an equivalence between the convex hull of \mathcal{G}' and the convex hull of the set \mathcal{F} with

$$\mathcal{F} = \{(1, x, X) : x \in \mathcal{X}, X = xx^\top\}.$$

Note, that in [13] they omit the constant 1 and write $\mathcal{F} = \{(x, xx^\top) : x \in \mathcal{X}\}$. For a better understanding, we stick to the notations of Theorem 1 with our definition of \mathcal{F} , including the constant 1.

Since the feasible set \mathcal{X} in \mathcal{G}' is, in contrast to \mathcal{F} , also intersected with the affine set \mathcal{L} , Theorem 1 can not be directly applied but needs some facial decomposition.

Proposition 2 (Proposition 3 in [13]). *Assume that $q(x) > 0$ over a non-empty and bounded set $\mathcal{X} \cap \mathcal{L} \subseteq \mathbb{R}^n$ and suppose that $\mathcal{L} = \{x \in \mathbb{R}^n : Cx = d\}$ for some $C \in \mathbb{R}^{p \times n}$ and $d \in \mathbb{R}^p$. Then,*

$$\begin{aligned} \text{conv}(\mathcal{G}') = \{ & (\rho, y, Y) : (\rho, y, Y) \in \rho \text{conv}(\mathcal{F}), \\ & \langle A, Y \rangle + a^\top y + a_0 \rho = 1, \rho \geq 0, \\ & \text{tr}(CYC^\top - Cyd^\top - dy^\top C^\top + \rho dd^\top) = 0 \}. \end{aligned}$$

For $\mathcal{L} = \mathbb{R}^n$, additionally $\text{conv}(\mathcal{F}) = \{(1, x, X) : (1, x, X) \in \sigma \text{conv}(G'), \sigma \geq 0\}$ holds.

Depending on \mathcal{X} , it still remains to characterize the convex hull of \mathcal{F} . In the case of $\mathcal{X} = \mathbb{R}_{\geq 0}^n$ for example, we have that $\mathcal{F} = \{(1, x, X) : x \in \mathbb{R}_{\geq 0}^n, X = xx^\top\}$ and hence the convex hull of \mathcal{F} is

$$\text{conv}(\mathcal{F}) = \left\{ (1, x, X) : \begin{pmatrix} X & x \\ x^\top & 1 \end{pmatrix} \in \mathcal{CP}^{n+1} \right\},$$

where \mathcal{CP}^{n+1} denotes the cone of completely positive matrices of dimension $(n+1) \times (n+1)$. This immediately allows us to state the following corollary.

Corollary 3 (Corollary 3 in [13]). *If \mathcal{X} is the non-negative orthant, and suppose that $\mathcal{L} = \{x \in \mathbb{R}^n : Cx = d\}$ for some $C \in \mathbb{R}^{p \times n}$ and $d \in \mathbb{R}^p$, then (4) can be formulated as*

$$\begin{aligned} \min \quad & \langle B, Y \rangle + b^\top y + b_0 \rho \\ \text{s.t.} \quad & \langle A, Y \rangle + a^\top y + a_0 \rho = 1 \\ & \text{tr}(CYC^\top - Cyd^\top - dy^\top C^\top + \rho dd^\top) = 0 \\ & \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} \in \mathcal{CP}^{n+1}. \end{aligned} \tag{6}$$

To handle binary variables in this setting, one can introduce non-negative slack variables \bar{z}_i for each original variable \bar{x}_i and require $\bar{x}_i + \bar{z}_i = 1$. We collect all these variables in a vector $x^\top = (\bar{x}^\top \ \bar{z}^\top)$. Let k be the index of \bar{z}_i in the variable vector x . Since we are working with completely positive matrices, it can be shown that by adding the constraint $X_{ik} = 0$, we get an exact reformulation, as every extreme ray belonging to the face implied by this constraint satisfies the binary condition, see Remark 4 in [13].

We are now ready to apply the theory of [13] presented in this section to the problem of computing the edge expansion of a graph.

3.2 Applying the convexification techniques to the edge expansion

In analogy to the general notation for the objective function of quadratic fractional problems from Section 3.1 above, we get that for the edge expansion problem $B = L$, $b = 0$, $b_0 = 0$, and $A = 0$, $a = e_n$, $a_0 = 0$. In the next two subsections, we give two different ways to reformulate (1). The first one is to apply Theorem 1 directly and the second one is to formulate the problem in such a way that Proposition 2 can be used.

3.2.1 Reformulation with Theorem 1

Referring to the notation from before, we define

$$\begin{aligned} \mathcal{G}' &= \left\{ \frac{(1, \bar{x}, \bar{x}\bar{x}^\top)}{e^\top \bar{x}} : \bar{x} \in \{0, 1\}^n, 1 \leq e^\top \bar{x} \leq \left\lfloor \frac{n}{2} \right\rfloor \right\}, \text{ and} \\ \mathcal{F}' &= \left\{ (1, \bar{x}, \bar{x}\bar{x}^\top) : \bar{x} \in \{0, 1\}^n, 1 \leq e^\top \bar{x} \leq \left\lfloor \frac{n}{2} \right\rfloor \right\}. \end{aligned}$$

With Theorem 1 we get that

$$\text{conv}(\mathcal{G}') = \left\{ (\rho, \bar{y}, \bar{Y}) : (\rho, \bar{y}, \bar{Y}) \in \rho \text{conv}(\mathcal{F}'), e^\top \bar{y} = 1, \rho \geq 0 \right\} \tag{7}$$

and $h(G) = \min\{\langle L, \bar{Y} \rangle : (\rho, \bar{y}, \bar{Y}) \in \text{conv}(\mathcal{G}')\}$ holds. Consequently, we are now interested in describing $\text{conv}(\mathcal{F}')$. Motivated by the proof of Proposition 2 in [13], we introduce the slack variables s and t to rewrite the linear inequalities as the equations

$$\underbrace{\begin{pmatrix} e_n^\top & 1 & 0 \\ e_n^\top & 0 & -1 \end{pmatrix}}_{\tilde{C}} \cdot \underbrace{\begin{pmatrix} \bar{x} \\ s \\ t \end{pmatrix}}_{\tilde{x}} = \underbrace{\begin{pmatrix} \lfloor \frac{n}{2} \rfloor \\ 1 \end{pmatrix}}_{\tilde{d}}.$$

It then holds that

$$\text{conv}(\mathcal{F}') = \left\{ (1, \tilde{x}, \tilde{X}) : \text{tr}(\tilde{C}\tilde{X}\tilde{C}^\top - \tilde{C}\tilde{x}\tilde{d}^\top - \tilde{d}\tilde{x}^\top\tilde{C}^\top + \tilde{d}\tilde{d}^\top) = 0, (1, \tilde{x}, \tilde{X}) \in \text{conv}(\mathcal{F}) \right\}$$

with

$$\mathcal{F} = \left\{ (1, \tilde{x}, \tilde{X}) : \tilde{X} = \tilde{x}\tilde{x}^\top, \tilde{x}^\top = (\bar{x}^\top \quad s \quad t), \bar{x} \in \{0, 1\}^n, s, t \in \mathbb{R}_{\geq 0} \right\},$$

where the details of the proof can be found in [13]. Let

$$\tilde{L} = \text{Diag}(L, 0_2),$$

then (1) is equivalent to

$$\begin{aligned} h(G) = \min \quad & \langle \tilde{L}, \tilde{Y} \rangle \\ \text{s.t.} \quad & (e_n^\top \quad 0_2^\top) \tilde{y} = 1 \\ & \text{tr}(\tilde{C}\tilde{Y}\tilde{C}^\top - \tilde{C}\tilde{y}\tilde{d}^\top - \tilde{d}\tilde{y}^\top\tilde{C}^\top + \rho\tilde{d}\tilde{d}^\top) = 0 \\ & (\rho, \tilde{y}, \tilde{Y}) \in \rho \text{conv}(\mathcal{F}) \\ & \rho \geq 0. \end{aligned} \tag{8}$$

The constraint $\text{tr}(\tilde{C}\tilde{Y}\tilde{C}^\top - \tilde{C}\tilde{y}\tilde{d}^\top - \tilde{d}\tilde{y}^\top\tilde{C}^\top + \rho\tilde{d}\tilde{d}^\top) = 0$ can also be written as the linear equality constraint

$$\left\langle \begin{pmatrix} \tilde{C}^\top \\ -\tilde{d}^\top \end{pmatrix} (\tilde{C} \quad -\tilde{d}), \begin{pmatrix} \tilde{Y} & \tilde{y} \\ \tilde{y}^\top & \rho \end{pmatrix} \right\rangle = 0$$

in the matrix variable and is, therefore, easy to handle. But still, the problem remains to optimize over the convex hull of \mathcal{F} .

In the next subsection, we use the more general Proposition 2 to rewrite (1) as a completely positive optimization problem.

3.2.2 Reformulation applying Proposition 2

Additionally to the slack variables $s, t \in \mathbb{R}_{\geq 0}$ for the two inequalities of (1), we now introduce for $\bar{x} \in \mathbb{R}_{\geq 0}^n$ the slack variables $\bar{z} \in \mathbb{R}_{\geq 0}^n$. We denote by x the vector collecting all variables, namely $x^\top = (\bar{x}^\top \quad \bar{z}^\top \quad s \quad t)$, and set

$$C = \begin{pmatrix} e_n^\top & 0_n^\top & 1 & 0 \\ e_n^\top & 0_n^\top & 0 & -1 \\ I_n & I_n & 0_n & 0_n \end{pmatrix} \in \mathbb{R}^{(n+2) \times (2n+2)} \quad \text{and} \quad d = \begin{pmatrix} \lfloor \frac{n}{2} \rfloor \\ 1 \\ e_n \end{pmatrix} \in \mathbb{R}^{n+2}$$

to formulate the affine set as $\mathcal{L} = \{x \in \mathbb{R}^{2n+2} : Cx = d\}$. We further set the matrix variable Y and the vector variable y to be of the form

$$Y = \begin{pmatrix} Y^{11} & Y^{12} & Y^{13} & Y^{14} \\ Y^{21} & Y^{22} & Y^{23} & Y^{24} \\ Y^{31} & Y^{32} & Y^{33} & Y^{34} \\ Y^{41} & Y^{42} & Y^{43} & Y^{44} \end{pmatrix} \in \mathcal{S}^{2n+2} \quad \text{and} \quad y = \begin{pmatrix} y^1 \\ y^2 \\ y^3 \\ y^4 \end{pmatrix} \in \mathbb{R}^{2n+2},$$

that is Y is a matrix given in block format with $Y^{11}, Y^{22} \in \mathcal{S}^n$ and $Y^{33}, Y^{44} \in \mathbb{R}$ and the vector y consists of $y^1, y^2 \in \mathbb{R}^n$ and $y^3, y^4 \in \mathbb{R}$. For convenience of referring to specific parts of the matrix/vector, the structure of $Y \in \mathcal{S}^{2n+2}$ and $y \in \mathbb{R}^{2n+2}$ is implicitly consistent throughout the rest of this paper.

By Proposition 2 and the remark after it holds that

$$\begin{aligned}
h(G) = \min \quad & \langle L, Y \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_n^\top \quad 0_2^\top)y = 1 \\
& \text{tr}(CYC^\top - Cyd^\top - dy^\top C^\top + \rho dd^\top) = 0 \\
& \text{diag}(Y^{12}) = 0 \\
& \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} \in \mathcal{CP}^{2n+3},
\end{aligned} \tag{9}$$

where $L = \text{Diag}(L, 0_{n+2})$ or $L = \frac{1}{2} \text{Diag}(I_2 \otimes L, 0_2)$. Note the similarity to the vector lifting procedure applied in [27] to the bisection problem. There, two vectors, each indicating the vertices in the first and second partition, respectively, are lifted into the space of $(2n+1) \times (2n+1)$.

In the following sections of this paper, we are going to consider the exact reformulation (9).

4 A DNN relaxation of the reformulated problem

To optimize over the cone of completely positive matrices is NP-hard. But we can use the fact that every completely positive matrix is doubly non-negative, i.e., it is positive semidefinite and its entries are non-negative, to derive a DNN relaxation of (9), which is

$$\begin{aligned}
\min \quad & \langle L, Y \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top)y = 1 \\
& \text{tr}(CYC^\top - Cyd^\top - dy^\top C^\top + \rho dd^\top) = 0 \\
& \text{diag}(Y^{12}) = 0 \\
& \tilde{Y} = \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} \in \text{DNN}.
\end{aligned} \tag{DNN-P}$$

Let $M = (C \quad -d)$, then we can rewrite the trace constraint in (DNN-P) as

$$\text{tr}(CYC^\top - Cyd^\top - dy^\top C^\top + \rho dd^\top) = \text{tr}(M\tilde{Y}M^\top) = \text{tr}(M^\top M\tilde{Y}) = 0.$$

One can easily see that there exists no positive definite matrix \tilde{Y} fulfilling the trace constraint, as for any positive definite matrix \tilde{Y} we have $\text{tr}(M\tilde{Y}M^\top) > 0$. Hence, (DNN-P) has no Slater point. To obtain strict feasibility and reduce the dimension of the matrix variable \tilde{Y} , we perform a facial reduction.

4.1 Facial reduction

In this section, we apply facial reduction to (DNN-P) in order to obtain a formulation with a Slater feasible point. For this, we first state the following helpful proposition, which is a variant of Proposition 1 in [5] but with ρ in the bottom-right corner of \tilde{Y} instead of 1.

Proposition 4. *Let $M = (C \quad -d)$ and*

$$\tilde{Y} = \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} \succeq 0,$$

then the following three statements are equivalent.

1. $Cy = \rho d$ and $\text{diag}(CYC^\top) = \rho d^2$, where the square is to be interpreted element-wise.
2. $M\tilde{Y}M^\top = 0$, or equivalently $\text{tr}(M\tilde{Y}M^\top) = 0$.
3. $M\tilde{Y} = 0$.

Proof. Assume that $Cy = \rho d$ and $\text{diag}(CYC^\top) = \rho d^2$ holds. Let c_i^\top denote the i -th row of C . It then holds that

$$(M\tilde{Y}M^\top)_{ii} = (c_i^\top \quad -d_i)\tilde{Y}\begin{pmatrix} c_i \\ -d_i \end{pmatrix} = c_i^\top Y c_i - 2d_i c_i^\top y + \rho d_i^2 = \rho d_i^2 - 2\rho d_i^2 + \rho d_i^2 = 0.$$

Hence, the diagonal and therefore also the trace of $M\tilde{Y}M^\top$ is zero. Since \tilde{Y} is positive semidefinite, also $M\tilde{Y}M^\top$ is positive semidefinite, leading to the conclusion that the equality $M\tilde{Y}M^\top = 0$ has to hold.

For the second part of the proof, assume that $\text{tr}(M\tilde{Y}M^\top) = 0$. Since $\tilde{Y} \succeq 0$, we can write $\tilde{Y} = UU^\top$ for some matrix U . Plugging in, we obtain

$$0 = \text{tr}(M\tilde{Y}M^\top) = \text{tr}(MUU^\top M^\top) = \|MU\|^2,$$

which is equivalent to $MU = 0$ and therefor $M\tilde{Y} = MUU^\top = 0$.

Finally, assume that $M\tilde{Y} = 0$ holds. To prove the equality $Cy = \rho d$, we take a closer look at the last column of $M\tilde{Y}$. The i -th entry in the last column is

$$0 = (c_i^\top \quad -d_i)\begin{pmatrix} y \\ \rho \end{pmatrix} = c_i^\top y - \rho d_i,$$

yielding the desired equality $Cy = \rho d$. From $M\tilde{Y} = 0$ we get that $M\tilde{Y}M^\top = 0$. To prove that $\text{diag}(CYC^\top) = \rho d^2$ holds, we consider the diagonal of $M\tilde{Y}M^\top$. For the i -th entry of the diagonal, it holds that

$$0 = (c_i^\top \quad -d_i)\tilde{Y}\begin{pmatrix} c_i \\ -d_i \end{pmatrix} = c_i^\top Y c_i - 2d_i c_i^\top y + \rho d_i^2 = c_i^\top Y c_i - \rho d_i^2.$$

Hence, $\text{diag}(CYC^\top)_i = c_i^\top Y c_i = \rho d_i^2$ holds, which closes the proof. \square

For the facial reduction of (DNN-P), let W be a matrix such that its columns form an orthonormal basis of the nullspace of M . It then holds that

$$\{\tilde{Y} \succeq 0 : M\tilde{Y} = 0\} = \{WRW^\top : R \succeq 0\}. \quad (10)$$

Lemma 5. *The vectors*

$$w_{n+1} = \begin{pmatrix} 0_n \\ e_n \\ \lfloor \frac{n}{2} \rfloor \\ -1 \\ 1 \end{pmatrix} \text{ and } w_i = \begin{pmatrix} u_i \\ -u_i \\ -1 \\ 1 \\ 0 \end{pmatrix} \text{ for } i \in \{1, \dots, n\}$$

form a basis of $\ker(M)$, where u_i is the i -th unit vector with entry 1 at position i and 0 everywhere else.

Proof. Since the rank of M is $n+2$, the dimension of $\ker(M)$ is $(2n+3) - (n+2) = n+1$. Moreover, it is easy to check that the vectors w_1, \dots, w_{n+1} are linearly independent and satisfy $Mw_i = 0$ for $i \in [n+1]$. \square

To obtain the required matrix $W \in \mathbb{R}^{(2n+3) \times (n+1)}$, one can take as columns of W the orthonormalized basis vectors from Lemma 5. We can then rewrite (DNN-P) as

$$\begin{aligned} \min \quad & \langle \tilde{L}, \tilde{Y} \rangle \\ \text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\ & \text{diag}(Y^{12}) = 0 \\ & \tilde{Y} = \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} = WRW^\top \succeq 0 \\ & R \succeq 0, \end{aligned} \quad (\text{DNN-PFR})$$

with $\tilde{L} = \text{Diag}(L, 0_{n+3})$. We will show later in this section in Proposition 13 that one can also equivalently set $\tilde{L} = \frac{1}{2} \text{Diag}(I_2 \otimes L, 0_3)$. The reformulation (DNN-PFR) is indeed a strictly feasible formulation of (DNN-P). To prove this, we apply the following result of Hu, Sotirov, and Wolkowicz [16] on the existence of a Slater feasible point for DNN relaxations.

Theorem 6 (Theorem 3.15 in [16]). *Let*

$$\mathcal{Q} = \left\{ x \in \mathbb{R}^{2n+2} : \mathcal{A} \left(\begin{pmatrix} xx^\top & x \\ x^\top & 1 \end{pmatrix} \right) = 0, x \geq 0 \right\},$$

where \mathcal{A} is a linear transformation, and suppose $\text{aff}(\text{conv}(\mathcal{Q})) = \mathcal{L}$ with $\dim(\mathcal{L}) = n$. Then there exist C with full row rank and d such that

$$\mathcal{L} = \{x \in \mathbb{R}^{2n+2} : Cx = d\}.$$

Let $M = (C \quad -d)$ and W be a matrix such that its columns form a basis of $\ker(M)$. Let further $\mathcal{J} = \{(i, j) : x_i x_j = 0 \ \forall x \in \mathcal{Q}\}$ and let \mathcal{J}^c be its complement. Then there exists a Slater point \hat{R} for the set

$$\hat{\mathcal{Q}}_R = \left\{ R \in \mathcal{S}^{n+1} : R \succeq 0, (WRW^\top)_{\mathcal{J}^c} \geq 0, (WRW^\top)_{\mathcal{J}} = 0, \mathcal{A}(WRW^\top) = 0 \right\}$$

of feasible points.

With the help of this, we can now state the following result on Slater feasibility.

Theorem 7. *Relaxation (DNN-PFR) has a Slater feasible point.*

Proof. Let $x^\top = (\bar{x}^\top \quad \bar{z}^\top \quad s \quad t)$, then

$$\begin{aligned} \mathcal{Q} &= \left\{ x \in \mathbb{R}_{\geq 0}^{2n+2} : \bar{x}_i \bar{z}_i = 0 \ \forall i \in [n], \bar{x} + \bar{z} = e_n, e_n^\top \bar{x} + s = \left\lfloor \frac{n}{2} \right\rfloor, e_n^\top \bar{x} - t = 1 \right\} \\ &= \left\{ x \in \mathbb{Z}_{\geq 0}^{2n+2} : \bar{x} + \bar{z} = e_n, e_n^\top \bar{x} + s = \left\lfloor \frac{n}{2} \right\rfloor, e_n^\top \bar{x} - t = 1 \right\} \\ &= \left\{ x \in \mathbb{Z}_{\geq 0}^{2n+2} : Cx = d \right\}. \end{aligned}$$

With Ghouila-Houri's characterization of totally unimodular matrices one can show that C is totally unimodular and hence $\text{conv}(\mathcal{Q}) = \{x \in \mathbb{R}_{\geq 0}^{2n+2} : Cx = d\}$. One can further show that

$$\text{aff}(\text{conv}(\mathcal{Q})) = \{x \in \mathbb{R}^{2n+2} : Cx = d\},$$

which follows from the fact that $\text{aff}(\{x \in \mathbb{R}^{2n+2} : Ax \leq b\}) = \{x \in \mathbb{R}^{2n+2} : A^-x = b^-\}$. From the constraints we can see that the index set \mathcal{J} (see Theorem 6) is $\mathcal{J} = \{(i, n+i) : 1 \leq i \leq n\} \cup \{(n+j, j) : 1 \leq j \leq n\}$. In $\mathcal{A}(X)$ we have the constraints $CX_{:, (2n+3)} = d$ and $X_{i, (n+i)} = 0$ for all $1 \leq i \leq n$. On the matrices of the form WRW^\top , the first type of constraints is redundant, since $M(WRW^\top)_{:, (2n+3)} = 0$ holds for all matrices R as the columns of W span the kernel of M .

The second kind of constraints is $WRW_{\mathcal{J}}^\top = 0$. Hence, by Theorem 6, there exists a matrix $\hat{R} \in \mathcal{S}^{n+1}$ such that $\hat{R} \succ 0$, $(W\hat{R}W^\top)_{\mathcal{J}^c} > 0$ and $(W\hat{R}W^\top)_{\mathcal{J}} = 0$. Let

$$\kappa = \sum_{i=1}^n (W\hat{R}W^\top)_{i, (2n+3)} > 0,$$

then $\frac{1}{\kappa}\hat{R}$ is a strictly feasible solution of (DNN-PFR). \square

Proposition 4 was not only helpful for the facial reduction, but we can also use it to identify several redundant constraints, as shown in the next section.

4.2 Properties of (DNN-P) and (DNN-PFR)

In this section, we state several properties of (DNN-P) and (DNN-PFR). Some of these properties are useful for the algorithm that we derive in Section 5.

As already mentioned, we make in particular use of the result from Proposition 4 stating that every feasible solution of (DNN-P) satisfies $M\tilde{Y} = 0$ and $M\tilde{Y}M^\top = 0$. Note, that for feasible solutions WRW^\top of (DNN-PFR) it holds that $MWRW^\top = 0$ and hence all results in this section apply to both \tilde{Y} and WRW^\top . The first result focuses on the last row/column of feasible matrices, in particular bounds on ρ and connections between the entries in y are given.

Proposition 8. *Every feasible point of (DNN-P) and (DNN-PFR) satisfies*

$$\frac{1}{\lfloor \frac{n}{2} \rfloor} \leq \rho \leq 1.$$

Moreover, it holds that $y^1 \leq \rho$, $y^2 \leq \rho$, $y^2 = \rho e_n - y^1$, $y^3 = \rho \lfloor \frac{n}{2} \rfloor - 1$, and $y^4 = 1 - \rho$.

Proof. From the last column of the matrix equality $M\tilde{Y} = 0$ it follows that $Cy = \rho d$ and hence

$$\begin{aligned} (e_n^\top \quad 0_n^\top \quad 1 \quad 0)y &= \rho \lfloor \frac{n}{2} \rfloor \\ (e_n^\top \quad 0_n^\top \quad 0 \quad -1)y &= \rho \\ (I_n \quad I_n \quad 0_n \quad 0_n)y &= \rho e_n \end{aligned}$$

holds. Remember, that for simplicity we denoted $y = (y^1 \quad y^2 \quad y^3 \quad y^4)$ with $y^1, y^2 \in \mathbb{R}^n$ and $y^3, y^4 \in \mathbb{R}$. From the constraint $e_n^\top y^1 = 1$ and the equations above, it follows that $y^3 = \rho \lfloor \frac{n}{2} \rfloor - 1$. By the non-negativity of y^3 , we get that $\rho \geq \frac{1}{\lfloor \frac{n}{2} \rfloor}$ has to hold. With the same argumentation, we get that $y^4 = 1 - \rho \geq 0$ holds for every feasible point, proving the claimed upper bound on ρ . From the last of the above derived constraints and non-negativity, we get $y^1 = \rho e_n - y^2 \geq 0$ and $y^2 = \rho e_n - y^1 \geq 0$, which implies that $y^1 \leq \rho$ and $y^2 \leq \rho$ has to be satisfied. \square

Similarly, we can show the following connections between the submatrices Y^{11} , Y^{22} and Y^{12} and the vectors y^1 and y^2 .

Proposition 9. *Every feasible solution \tilde{Y} of (DNN-P) and (DNN-PFR) satisfies*

$$\begin{aligned} Y_{ij}^{11} + (Y^{12})_{ij}^\top &= y_j^1 \quad \text{and} \\ Y_{ij}^{22} + Y_{ij}^{12} &= y_j^2 \end{aligned}$$

for all $1 \leq i, j \leq n$.

Proof. By considering the equations

$$\begin{aligned} 0 &= (M\tilde{Y})_{(2n+i),j} = Y_{ij}^{11} + Y_{ij}^{21} - y_j^1 \quad \text{and} \\ 0 &= (M\tilde{Y})_{(2n+i),(n+j)} = Y_{ij}^{12} + Y_{ij}^{22} - y_j^2 \end{aligned}$$

for $1 \leq i, j \leq n$, one immediately obtains the above stated result. \square

We can further show that the bounds on the sum of the entries in Y^{11} are already implied by the constraints in (DNN-P) and (DNN-PFR) as well.

Proposition 10. *Every feasible point of (DNN-P) and (DNN-PFR) satisfies*

$$1 \leq \langle E, Y^{11} \rangle \leq \lfloor \frac{n}{2} \rfloor.$$

Proof. From the positive semidefiniteness of the matrix variable, it follows that

$$\begin{aligned} 0 &\leq \begin{pmatrix} e_n^\top & 0_{n+2}^\top & -1 \end{pmatrix} \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix} \begin{pmatrix} e_n \\ 0_{n+2} \\ -1 \end{pmatrix} \\ &= e_n^\top Y^{11} e_n - 2(e_n^\top \ 0_{n+2}^\top)^\top y + \rho \\ &= \langle E, Y^{11} \rangle - 2 + \rho. \end{aligned}$$

Since $\rho \leq 1$, we obtain the lower bound $1 \leq \langle E, Y^{11} \rangle$.

Considering Proposition 8 and

$$0 = (M\tilde{Y})_{1,(2n+1)} = e_n^\top Y^{13} + Y^{33} - \lfloor \frac{n}{2} \rfloor y^3 = e_n^\top Y^{13} + Y^{33} - \lfloor \frac{n}{2} \rfloor^2 \rho + \lfloor \frac{n}{2} \rfloor,$$

yields

$$e_n^\top Y^{13} + Y^{33} = \lfloor \frac{n}{2} \rfloor^2 \rho - \lfloor \frac{n}{2} \rfloor.$$

Plugging this into $(M\tilde{Y}M^\top)_{1,1} = 0$, we can then derive

$$\begin{aligned} 0 &= e_n^\top Y^{11} e_n + Y^{33} + \lfloor \frac{n}{2} \rfloor^2 \rho + 2e_n^\top Y^{13} - 2\lfloor \frac{n}{2} \rfloor e_n^\top y^1 - 2\lfloor \frac{n}{2} \rfloor y^3 \\ &= e_n^\top Y^{11} e_n + Y^{33} + \lfloor \frac{n}{2} \rfloor^2 \rho + 2e_n^\top Y^{13} - 2\lfloor \frac{n}{2} \rfloor - 2\lfloor \frac{n}{2} \rfloor \left(\lfloor \frac{n}{2} \rfloor \rho - 1 \right) \\ &= e_n^\top Y^{11} e_n + Y^{33} + 2e_n^\top Y^{13} - \lfloor \frac{n}{2} \rfloor^2 \rho \\ &= e_n^\top Y^{11} e_n + e_n^\top Y^{13} - \lfloor \frac{n}{2} \rfloor. \end{aligned}$$

Due to the non-negativity, it holds that $e_n^\top Y^{13} \geq 0$ and therefore $\langle E, Y^{11} \rangle \leq \lfloor \frac{n}{2} \rfloor$. \square

In addition to the non-negativity, we can derive the following upper bounds on the entries of all feasible matrices.

Proposition 11. *Every feasible solution of (DNN-P) and (DNN-PFR) satisfies*

$$\begin{aligned}
y^3 &\leq \left\lfloor \frac{n}{2} \right\rfloor - 1, \\
y^4 &\leq 1 - \frac{1}{\left\lfloor \frac{n}{2} \right\rfloor}, \\
Y^{33} &\leq \left\lfloor \frac{n}{2} \right\rfloor^2 - \left\lfloor \frac{n}{2} \right\rfloor, \\
Y^{44} &\leq \left\lfloor \frac{n}{2} \right\rfloor - 1, \\
Y^{34} &\leq \left\lfloor \frac{n}{2} \right\rfloor - 1, \\
Y^{13}, Y^{23} &\leq \left\lfloor \frac{n}{2} \right\rfloor - 1, \text{ and} \\
Y^{14}, \hat{Y}^{24} &\leq 1 - \frac{1}{\left\lfloor \frac{n}{2} \right\rfloor}.
\end{aligned}$$

Proof. The first two inequalities follow directly from Proposition 8, namely

$$\begin{aligned}
y^3 &= \rho \left\lfloor \frac{n}{2} \right\rfloor - 1 \leq \left\lfloor \frac{n}{2} \right\rfloor - 1 \text{ and} \\
y^4 &= 1 - \rho \leq 1 - \frac{1}{\left\lfloor \frac{n}{2} \right\rfloor}.
\end{aligned}$$

From $0 = (M\tilde{Y})_{1,(2n+1)} = e_n^\top Y^{13} + Y^{33} - \left\lfloor \frac{n}{2} \right\rfloor y^3$, we obtain

$$Y^{33} = \left\lfloor \frac{n}{2} \right\rfloor y^3 - e_n^\top Y^{13} \leq \left\lfloor \frac{n}{2} \right\rfloor^2 - \left\lfloor \frac{n}{2} \right\rfloor,$$

using the upper bound on y^3 and $Y \geq 0$. Similarly, we can derive the upper bound for Y^{34} . It holds that $0 = (M\tilde{Y})_{1,(2n+2)} = e_n^\top Y^{14} + Y^{34} - \left\lfloor \frac{n}{2} \right\rfloor y^4$, hence

$$Y^{34} = \left\lfloor \frac{n}{2} \right\rfloor y^4 - e_n^\top Y^{14} \leq \left\lfloor \frac{n}{2} \right\rfloor - 1.$$

For the upper bound on Y^{44} , consider the equations

$$\begin{aligned}
0 &= (M\tilde{Y})_{2,(2n+2)} = e_n^\top Y^{14} - Y^{44} - y^4 \Leftrightarrow e_n^\top Y^{14} = Y^{44} + y^4 \\
0 &= (M\tilde{Y}M^\top)_{2,2} = \langle E, Y^{11} \rangle + Y^{44} + \rho - 2e_n^\top Y^{14} - 2 + 2y^4.
\end{aligned}$$

Plugging in the first into the second equation, we get

$$Y^{44} = \langle E, Y^{11} \rangle + \rho - 2 \leq \left\lfloor \frac{n}{2} \right\rfloor - 1,$$

since $\langle E, Y^{11} \rangle \leq \left\lfloor \frac{n}{2} \right\rfloor$ (cf. Proposition 10) and $\rho \leq 1$. Next, observe that

$$\begin{aligned}
0_n &= (M\tilde{Y})_{3:(n+2),(2n+1)} = Y^{13} + Y^{23} - y^3 e_n \text{ and} \\
0_n &= (M\tilde{Y})_{3:(n+2),(2n+2)} = Y^{14} + Y^{24} - y^4 e_n
\end{aligned}$$

imply that $(Y^{13} + Y^{23})_i = y^3$ and $(Y^{14} + Y^{24})_i = y^4$ has to hold for all $i \in [n]$. Due to the non-negativity of Y , each of the summands on the left-hand side is bounded by the right-hand side of the equations. \square

We have already shown that Y^{11} and ρ satisfy the inequality constraints of the basic relaxation (DNN $_{n+1}$). In the subsequent section, we now want to strengthen our new relaxation (DNN-P) with further valid (in)equalities and compare it to the basic relaxation.

4.3 Strengthening and comparison to the basic DNN relaxation

Recall, that the constraint $\tilde{Y} \in \text{DNN}$ is the relaxation of $\tilde{Y} \in \mathcal{CP}^{2n+3}$, which is equivalent to $(\rho, y, Y) \in \rho \text{conv}(\{(1, x, xx^\top) : x \in \mathbb{R}_{\geq 0}^{2n+2}\})$, where we set $x^\top = (\bar{x}^\top \ \bar{z}^\top \ s \ t)$. Since the variables \bar{x} and \bar{z} are supposed to be binary, we can add the following diagonal constraints.

$$\text{diag}(Y^{11}) = y^1, \quad \text{diag}(Y^{22}) = y^2. \quad (11)$$

These constraints can be added to (DNN-PFR) without losing strict feasibility, as presented in the following proposition.

Proposition 12. *Relaxation (DNN-PFR) with the additional diagonal constraints (11) has a Slater feasible point.*

Proof. Note, that in the proof of Theorem 7 we can add to the description of \mathcal{Q} the constraint $\bar{x}_i \bar{x}_i = \bar{x}_i$ and $\bar{z}_i \bar{z}_i = \bar{z}_i$ for all $1 \leq i \leq n$ without any impact on $\text{aff}(\text{conv}(\mathcal{Q}))$. Hence, (DNN-PFR) with the diagonal constraint (11) has a Slater feasible point as well. \square

To be able to compare (DNN-P) to the basic relaxation (DNN $_{n+1}$), we first present the following result on the objective function.

Proposition 13. *Every feasible point \tilde{Y} of (DNN-P) and (DNN-PFR) satisfies*

$$Y^{22} = Y^{11} + \rho E - e_n (y^1)^\top - y^1 e_n^\top$$

and therefore

$$\langle Y, \text{Diag}(L, 0_{n+2}) \rangle = \frac{1}{2} \langle Y, \text{Diag}(I_2 \otimes L, 0_2) \rangle.$$

Proof. Using Proposition 9 and then Proposition 8, we get

$$\begin{aligned} Y_{ij}^{11} + Y_{ji}^{11} - Y_{ij}^{22} - Y_{ji}^{22} &= y_j^1 - Y_{ji}^{12} + y_i^1 - Y_{ij}^{12} - y_j^2 + Y_{ij}^{12} - y_i^2 + Y_{ji}^{12} \\ &= y_j^1 + y_i^1 - (\rho - y_j^1) - (\rho - y_i^1). \end{aligned}$$

From the symmetry of \tilde{Y} it follows that $Y^{11}, Y^{22} \in \mathcal{S}^n$ and hence,

$$Y_{ij}^{22} = Y_{ij}^{11} + \rho - y_i^1 - y_j^1.$$

It then holds that $\langle L, Y^{22} \rangle = \langle L, Y^{11} \rangle$ due to the properties of the Laplacian matrix L , which closes our proof. \square

Theorem 14. *Relaxation (DNN-P) with the diagonal constraint*

$$\text{diag}(Y^{11}) = y^1 \quad (12)$$

is at least as good as (DNN_{n+1}).

Proof. To prove the theorem, we construct for every feasible point of the formulation (DNN-P) + (12) a feasible point for (DNN_{n+1}) with the same objective function value. Let $\tilde{Y} \in \mathcal{S}^{2n+3}$ be a matrix satisfying all constraints in (DNN-P) and (12). From Propositions 8 and 10 and the constraint (12), we get that the submatrix

$$\begin{pmatrix} Y^{11} & y^1 \\ (y^1)^\top & \rho \end{pmatrix}$$

satisfies all constraints of (DNN_{n+1}). Due to Proposition 13, it holds that the objective function values are the same and hence (DNN-P) is at least as good as (DNN_{n+1}). \square

Remark 15. *Theorem 14 also works without adding the constraint $\text{diag}(Y^{11}) = y^1$ if we remove the constraint $\text{diag}(\tilde{Y}) = \bar{y}$ from (DNN_{n+1}), i.e., (DNN-P) is at least as good as (DNN_{n+1}) without the diagonal constraint.*

With the same argumentation as for the diagonal constraints, we can further strengthen relaxation (DNN-P) by adding scaled facet defining inequalities for the boolean quadric polytope (BQP) on y^1, y^2 and the left upper $2n \times 2n$ block of \tilde{Y} . The scaled (multiplied with ρ) BQP inequalities are

$$Y_{ij} \leq y_i \quad (13a)$$

$$Y_{ij} + Y_{ik} - Y_{jk} \leq y_i \quad (13b)$$

$$y_i + y_j - Y_{ij} \leq \rho \quad (13c)$$

$$y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} \leq \rho \quad (13d)$$

for all $1 \leq i, j, k \leq 2n$. Indeed, similarly as in [26] for the vector-lifted DNN relaxation of the graph bisection problem, we can show that constraints (13a) and (13c) are already implied by the constraints in (DNN-P) and (DNN-PFR).

Proposition 16. *Every feasible solution \tilde{Y} of (DNN-P) and (DNN-PFR) satisfies the scaled BQP inequalities (13a) and (13c).*

Proof. From Proposition 9 and $\tilde{Y} \geq 0$ it follows that $Y_{ij} \leq y_j$ for all $1 \leq i, j \leq 2n$, which is (13a).

By Proposition 13 and $Y^{22} \geq 0$ we get that $Y_{ij}^{11} + \rho - y_i^1 - y_j^1 \geq 0$ holds, which is equivalent to (13c) for $1 \leq i, j \leq n$. For $1 \leq i \leq n$ and $(n+1) \leq j \leq 2n$, let $k = j - n$, then (13c) can be written as

$$\rho \geq y_i^1 + y_k^2 - Y_k^{12} = y_i^1 + Y_{ik}^{22} = Y_{ik}^{11} - y_k^1 + \rho,$$

where the first equality follows from Proposition 9 and the second follows from Proposition 13. Hence, for this choice of i and j , (13c) is equivalent to (13a). In the same way,

one can prove the case $(n+1) \leq i \leq 2n$ and $1 \leq j \leq n$. For the case $(n+1) \leq i, j \leq 2n$ let $k = n - i$ and $\ell = n - j$. Applying Proposition 8 and Proposition 13 we obtain that (13c) can be written as

$$\rho \geq y_k^2 + y_\ell^2 - Y_{k\ell}^{22} = 2\rho - y_k^1 - y_\ell^1 - Y_{k\ell}^{22} = \rho - Y_{k\ell}^{11},$$

which is equivalent to $Y^{11} \geq 0$ and thus valid for every feasible solution of (DNN-P) and (DNN-PFR). \square

Corollary 17. *Relaxation (DNN-P) with the diagonal constraint*

$$\text{diag}(Y^{11}) = y^1$$

is at least as good as (DNN_{n+1}) with the additional constraints

$$\begin{aligned} \bar{Y}_{ij} &\leq \bar{y}_i \\ \bar{y}_i + \bar{y}_j - \bar{Y}_{ij} &\leq \rho \end{aligned}$$

for $1 \leq i, j \leq n$.

Proof. The statement follows from the proof of Theorem 14 and Proposition 16. \square

Our numerical tests suggest that (13b) leads to a better improvement of the DNN relaxation than (13d). The diagonal constraint yields a small improvement only, and therefore we will not consider it for our relaxation.

Solving the relaxation with non-negativity and scaled triangle inequalities with interior point solvers in a reasonable time is not possible due to the number of constraints. In the next section, we therefore introduce an augmented Lagrangian algorithm to compute the strengthened DNN relaxation.

5 Solving the DNN relaxation

5.1 An augmented Lagrangian algorithm

Problem (DNN-PFR) strengthened by a subset \mathcal{T} of the scaled BQP inequalities (13b) can be written as

$$\begin{aligned} \min \quad & \langle W^\top \tilde{L}W, R \rangle \\ \text{s.t.} \quad & \mathcal{A}(WRW^\top) = b \\ & \mathcal{B}(WRW^\top) \leq 0 && \text{(DNN-PFRC)} \\ & WRW^\top \geq 0 \\ & R \succeq 0, \end{aligned}$$

where $\mathcal{A}: \mathcal{S}^{2n+3} \rightarrow \mathbb{R}^p$ is the operator corresponding to the linear equality constraints from (DNN-PFR) and $\mathcal{B}: \mathcal{S}^{2n+3} \rightarrow \mathbb{R}^q$ is the operator corresponding to the BQP inequalities in \mathcal{T} . Note that p denotes the number of equality constraints and is equal to $3n+1$

if the diagonal constraint is included and $n + 1$ otherwise. The number of BQP inequalities in \mathcal{T} is denoted by q . We define the Lagrangian function with respect to the primal variable $R \succeq 0$ and the dual variables $\nu \in \mathbb{R}^p$, $\mu \in \mathbb{R}^q$, $S \in \mathcal{S}^{2n+3}$ and $Z \in \mathcal{S}^{n+1}$ corresponding to the equality constraints, inequality constraints, non-negativity and positive semidefiniteness constraint, as

$$\begin{aligned}\mathcal{L}(R; \nu, \mu, S, Z) &= \langle W^\top \tilde{L}W, R \rangle + \nu^\top (b - \mathcal{A}(WRW^\top)) + \mu^\top \mathcal{B}(WRW^\top) \\ &\quad - \langle WRW^\top, S \rangle - \langle R, Z \rangle \\ &= b^\top \nu - \langle W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z, R \rangle.\end{aligned}$$

The Lagrange dual function is then defined by

$$g(\nu, \mu, S, Z) = \inf_{R \in \mathcal{S}^{n+1}} \mathcal{L}(R; \nu, \mu, S, Z) = \begin{cases} b^\top \nu & \text{if } W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z = 0, \\ -\infty & \text{else,} \end{cases}$$

and the dual problem of (DNN-PFRC) is given by $\max_{\nu, \mu \geq 0, S \geq 0, Z \succeq 0} g(\nu, \mu, S, Z)$, that is

$$\begin{aligned}\max \quad & b^\top \nu \\ \text{s.t.} \quad & W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z = 0 \\ & \nu \in \mathbb{R}^p, \mu \geq 0, S \geq 0, Z \succeq 0.\end{aligned} \tag{DNN-DFRC}$$

We propose to use the augmented Lagrangian approach to approximately solve the above dual problem. By introducing a Lagrange multiplier R for the dual equality constraint, and a penalty parameter $\alpha > 0$, the augmented Lagrangian function \mathcal{L}_α can be written as

$$\begin{aligned}\mathcal{L}_\alpha(\nu, \mu, S, Z; R) &= b^\top \nu - \langle W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z, R \rangle \\ &\quad - \frac{1}{2\alpha} \left\| W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z \right\|^2 \\ &= b^\top \nu - \frac{1}{2\alpha} \left\| W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L})W + Z + \alpha R \right\|^2 + \frac{\alpha}{2} \|R\|^2.\end{aligned}$$

Note that the Lagrangian dual of (DNN-DFRC) is again (DNN-PFRC), which justifies our choice of the dual variable name R . The augmented Lagrangian method for solving (DNN-DFRC) consists in maximizing $\mathcal{L}_\alpha(\nu, \mu, S, Z; R_k)$ for a fixed $\alpha > 0$ and R_k to get $\nu_k \in \mathbb{R}^p$, $\mu_k \geq 0$, $S_k \geq 0$ and $Z_k \succeq 0$. Then the primal matrix R is updated using

$$R_{k+1} = R_k - \frac{1}{\alpha} (W^\top (\mathcal{A}^\top \nu_k - \mathcal{B}^\top \mu_k + S_k - \tilde{L})W + Z_k), \tag{14}$$

see [2]. By construction, the primal matrix \tilde{Y} is then given by

$$\tilde{Y} = WRW^\top. \tag{15}$$

In the augmented Lagrangian method, as opposed to the penalty method, the penalty parameter α does not necessarily need to go to zero in order to guarantee convergence.

However, to avoid problem-specific tuning of the penalty parameter, we let $\alpha \rightarrow 0$. Decreasing α makes the subproblem in each iteration harder to solve due to ill-conditioning. First-order methods are particularly sensitive to ill-conditioning, hence, we use here a quasi-Newton method to solve the inner problem.

For given $\alpha > 0$ and $R \succeq 0$, the inner maximization problem

$$\begin{aligned} \max \quad & b^\top \nu - \frac{1}{2\alpha} \left\| W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + Z + \alpha R \right\|^2 + \frac{\alpha}{2} \|R\|^2 \\ \text{s.t.} \quad & \nu \in \mathbb{R}^p, \mu \geq 0, S \geq 0, Z \succeq 0 \end{aligned} \quad (16)$$

can be further simplified by eliminating the matrix Z as follows. Define

$$M = W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R.$$

For fixed ν, μ and S , the optimal Z of problem (16) is the same as

$$\arg \min_{Z \succeq 0} \|Z + M\|^2,$$

which is the projection of $-M$ onto the cone of positive semidefinite matrices. It is well known that the solution $Z = \mathcal{P}_{\succeq 0}(-M) = -\mathcal{P}_{\preceq 0}(M)$ can be computed from the eigenvalue decomposition of M , see [14].

By eliminating Z in (16) we get

$$\begin{aligned} \max \quad & b^\top \nu - \frac{1}{2\alpha} \left\| \mathcal{P}_{\succeq 0}(W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R) \right\|^2 + \frac{\alpha}{2} \|R\|^2 \\ \text{s.t.} \quad & \nu \in \mathbb{R}^p, \mu \geq 0, S \geq 0. \end{aligned} \quad (17)$$

Let $F_\alpha(\nu, \mu, S)$ denote the objective function of (17). We can then state the following properties of the objective function.

Proposition 18. *Let $\alpha > 0$ and $F_\alpha(\nu, \mu, S)$ be the objective function of (17). The function $F_\alpha(\nu, \mu, S)$ is concave and differentiable, with partial gradients given by*

$$\begin{aligned} \nabla_S F_\alpha(\nu, \mu, S) &= -\frac{1}{\alpha} W \mathcal{P}_{\succeq 0}(W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R) W^\top, \\ \nabla_{\nu_i} F_\alpha(\nu, \mu, S) &= b_i - \frac{1}{\alpha} \left\langle A_i, W \mathcal{P}_{\succeq 0}(W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R) W^\top \right\rangle \\ \nabla_{\mu_j} F_\alpha(\nu, \mu, S) &= \frac{1}{\alpha} \left\langle B_j, W \mathcal{P}_{\succeq 0}(W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R) W^\top \right\rangle \end{aligned}$$

for all $1 \leq i \leq p$, and $1 \leq j \leq q$.

Proof. Let $f: \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ be defined by $f(x) = \frac{1}{2} \|x_+\|^2$, where x_+ is the vector of length $n+1$ with $(x_+)_i = \max(0, x_i)$. Then f is a convex and differentiable function with gradient $\nabla f(x) = x_+$. Note that the objective function F_α can be written as

$$F_\alpha(\nu, \mu, S) = b^\top \nu - \frac{1}{\alpha} g \left(W^\top (\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \tilde{L}) W + \alpha R \right) + \frac{\alpha}{2} \|R\|^2$$

where the function $g: \mathcal{S}^{n+1} \rightarrow \mathbb{R}$ is defined by

$$g(X) = \frac{1}{2} \|\mathcal{P}_{\geq 0}(X)\|^2 = \frac{1}{2} \sum_{i=1}^{n+1} (\max(0, \lambda_i(X)))^2 = f(\lambda(X)),$$

where $\lambda(X)$ denotes the vector containing all eigenvalues of X . From [4, §5.2] we have that the function g is convex and differentiable with gradient $\nabla g(X) = \mathcal{P}_{\geq 0}(X)$. Hence, we can conclude that F_α is concave and differentiable.

To obtain the gradients, we apply the chain rule. For this, let $D_1, D_2, D_3 \in \mathcal{S}^{n+1}$ where D_1 is independent of ν , D_2 is independent of μ and D_3 is independent of S . Let further $\mathcal{M}_1: \mathbb{R}^p \rightarrow \mathcal{S}^{n+1}$, $\mathcal{M}_2: \mathbb{R}^q \rightarrow \mathcal{S}^{n+1}$ and $\mathcal{N}: \mathcal{S}^{2n+3} \rightarrow \mathcal{S}^{n+1}$ be linear operators defined by

$$\begin{aligned} \mathcal{M}_1 \nu &= W^\top (A^\top \nu) W = \sum_{i=1}^p \nu_i (W^\top A_i W), \\ \mathcal{M}_2 \mu &= W^\top (B^\top \mu) W = \sum_{j=1}^q \mu_j (W^\top B_j W) \text{ and} \\ \mathcal{N}(S) &= W^\top S W. \end{aligned}$$

Their adjoints are $(\mathcal{M}_1^* X)_i = \langle W^\top A_i W, X \rangle$, $(\mathcal{M}_2^* X)_j = \langle W^\top B_j W, X \rangle$ and $\mathcal{N}^*(X) = W X W^\top$, respectively. Now, applying the chain rule, we get

$$\begin{aligned} \nabla_\nu [g(\mathcal{M}_1 \nu + D_1)] &= \mathcal{M}_1^* \nabla g(\mathcal{M}_1 \nu + D_1), \\ \nabla_\mu [g(-\mathcal{M}_2 \mu + D_2)] &= -\mathcal{M}_2^* \nabla g(-\mathcal{M}_2 \mu + D_2) \text{ and} \\ \nabla_S [g(\mathcal{N}(S) + D_3)] &= \mathcal{N}^* \nabla g(\mathcal{N}(S) + D_3), \end{aligned}$$

verifying our stated gradients. □

Using this proposition allows that for a fixed $\alpha > 0$ and R the function $-F_\alpha$ is minimized using the L-BFGS-B algorithm [6].

To make the algorithm efficient in practice, for a fixed set of cuts \mathcal{T} and α , we perform only one iteration of the augmented Lagrangian method, i.e., we approximately solve the inner problem (17), update R by (14), and proceed to search for new violated inequalities in WRW^\top and add them to \mathcal{T} . If we find no or only a few violations, we reduce α and repeat until the penalty parameter α is smaller than a certain threshold. At the end, we perform several augmented Lagrangian iterations with the same α and without adding new cuts.

A similar solution technique was also used in [19], where the penalty method is applied to the dual problem and the resulting nonlinear function is minimized using a quasi-Newton method, and in [15], where the augmented Lagrangian method is used to solve an SDP relaxation strengthened by cutting planes. We have extended this methodology to facially reduced DNN programs.

5.2 Post processing to derive a valid lower bound

Our approach yields a dual solution (ν, μ, S, Z) of moderate precision. In particular, the constraint $W^\top(\mathcal{A}^\top\nu - \mathcal{B}^\top\mu + S - \tilde{L})W + Z = 0$ does not necessarily hold. However, because of weak duality, every feasible solution of the dual (DNN-DFRC) gives a lower bound on the optimal value of (DNN-PFRC). To derive a safe dual lower bound, we adapt the methods of [7] and [17], where the post-processing of [17] is for SDPs and was adapted by [7] for DNNs. Both approaches are based on the following Lemma.

Lemma 19 (Lemma 3.1 in [17]). *Let $A, B \in \mathcal{S}^{2n+3}$ with*

$$\underline{b} \leq \lambda_{\min}(B), \quad 0 \leq \lambda_{\min}(A), \quad \lambda_{\max}(A) \leq \bar{a}$$

for some $\underline{b}, \bar{a} \in \mathbb{R}$. Then the inequality

$$\langle A, B \rangle \geq \bar{a} \sum_{i: \lambda_i(B) < 0} \lambda_i(B) \geq \bar{a}(2n+3) \min\{0, \underline{b}\}$$

holds.

This leads us to the following theorem of [17, 7] adapted for facially reduced DNNs.

Theorem 20. *Consider the facially reduced primal problem (DNN-PFRC), let R^* be an optimal solution and let p^* be its optimal value. Given $\nu \in \mathbb{R}^p$, $\mu \in \mathbb{R}^q$ and $S \in \mathcal{S}^{2n+3}$ with $\mu \geq 0$ and $S \geq 0$, set*

$$\tilde{Z} = W^\top(\tilde{L} - \mathcal{A}^\top\nu + \mathcal{B}^\top\mu - S)W$$

and suppose that $\underline{z} \leq \lambda_{\min}(W\tilde{Z}W^\top)$. Assume $\bar{r} \in \mathbb{R}$ such that $\bar{r} \geq \lambda_{\max}(WR^*W^\top)$ is known. Then the inequality

$$p^* \geq b^\top\nu + \bar{r} \sum_{i: \lambda_i(W\tilde{Z}W^\top) < 0} \lambda_i(W\tilde{Z}W^\top) \geq b^\top\nu + \bar{r}(2n+3) \min\{0, \underline{z}\} \quad (18)$$

holds.

Proof. Let R^* be optimal for (DNN-PFRC), then

$$\begin{aligned} \langle W^\top\tilde{L}W, R^* \rangle - b^\top\nu &= \langle \tilde{L}, WR^*W^\top \rangle - \langle \mathcal{A}(WR^*W^\top), \nu \rangle \\ &= \langle \tilde{L} - \mathcal{A}^\top\nu, WR^*W^\top \rangle \\ &= \langle W^\top(\tilde{L} - \mathcal{A}^\top\nu)W, R^* \rangle \\ &= \langle W^\top(S - \mathcal{B}^\top\mu)W + \tilde{Z}, R^* \rangle \\ &= \langle S, WR^*W^\top \rangle - \langle \mathcal{B}^\top\mu, WR^*W^\top \rangle + \langle \tilde{Z}, R^* \rangle \\ &\geq -\langle \mathcal{B}^\top\mu, WR^*W^\top \rangle + \langle \tilde{Z}, R^* \rangle \\ &= -\mu^\top\mathcal{B}(WR^*W^\top) + \langle \tilde{Z}, R^* \rangle \\ &\geq \langle \tilde{Z}, R^* \rangle \end{aligned}$$

holds, where the first inequality follows from the fact that $S \geq 0$ and $WR^*W^\top \geq 0$, and the second inequality follows from the fact that $\mu \geq 0$ and $\mathcal{B}(WR^*W^\top) \leq 0$. Consequently, with Lemma 19 the inequality

$$\begin{aligned} p^* &= \langle W^\top \tilde{L}W, R^* \rangle \\ &\geq b^\top \nu + \langle \tilde{Z}, R^* \rangle \\ &= b^\top \nu + \langle W \tilde{Z}W^\top, WR^*W^\top \rangle \\ &\geq b^\top \nu + \bar{r} \sum_{i: \lambda_i(W \tilde{Z}W^\top) < 0} \lambda_i(W \tilde{Z}W^\top) \geq b^\top \nu + \bar{r}(2n+3) \min\{0, \underline{z}\} \end{aligned}$$

holds. \square

Given that we know an upper bound on the largest eigenvalue of WR^*W^\top , where R^* is an optimal solution of (DNN-PFRC) and hence also feasible for (DNN-PFR), we can compute a safe lower bound on (DNN-PFRC) by applying Theorem 20 in a post-processing step. To this end, we state an upper bound on the largest eigenvalue of all feasible solutions \tilde{Y} of (DNN-PFR) in the next Proposition. Again, note that $WR^*W^\top = \tilde{Y}^*$ is optimal for (DNN-P) under the assumption that R^* is optimal for (DNN-PFR).

Proposition 21. *Let $\tilde{Y} = WRW^\top$ be a feasible solution of (DNN-PFR), then*

$$\lambda_{\max}(\tilde{Y}) \leq \text{tr}(\tilde{Y}) \leq \left\lfloor \frac{n}{2} \right\rfloor^2 + n$$

holds.

Proof. Since the matrix \tilde{Y} is positive semidefinite, its eigenvalues are non-negative and therefore the trace gives an upper bound on the largest eigenvalue.

From Propositions 8 and 11 we already know that $\rho \leq 1$ and $Y^{33} + Y^{44} \leq \left\lfloor \frac{n}{2} \right\rfloor^2 - 1$ holds for every feasible solution. For the submatrices Y^{11} and Y^{22} of \tilde{Y} , consider for $i \in [n]$ the equations

$$0 = (M\tilde{Y}M^\top)_{2+i,2+i} = Y_{ii}^{11} + Y_{ii}^{22} + \rho + 2Y_{ii}^{12} - 2y_i^1 - 2y_i^2.$$

Since $Y_{ii}^{12} = 0$, this yields the equality $Y_{ii}^{11} + Y_{ii}^{22} = 2(y_i^1 + y_i^2) - \rho$. Summing over all indices $i \in [n]$ gives

$$\begin{aligned} \text{tr}(Y^{11}) + \text{tr}(Y^{22}) &= \sum_{i=1}^n (Y_{ii}^{11} + Y_{ii}^{22}) = 2(e_n^\top y^1 + e_n^\top y^2) - n\rho \\ &= 2(e_n^\top y^1 + e_n^\top (\rho e_n - y^1)) - n\rho = n\rho, \end{aligned}$$

where we used the equality $y^2 = \rho e_n - y^1$ from Proposition 8. To sum up, we obtain

$$\begin{aligned} \text{tr}(\tilde{Y}) &= \text{tr}(Y^{11}) + \text{tr}(Y^{22}) + Y^{33} + Y^{44} + \rho \\ &\leq (n+1)\rho + \left\lfloor \frac{n}{2} \right\rfloor^2 - 1 \leq \left\lfloor \frac{n}{2} \right\rfloor^2 + n, \end{aligned}$$

which is the claimed upper bound. \square

We summarize our bounding routine in Algorithm 1. Note that separating the BQP inequalities (13b) can be done in $\mathcal{O}(n^3)$ by complete enumeration.

Algorithm 1 Computation of DNN bound with BQP inequalities

input: $\alpha > 0$, matrices \tilde{L} , W , initial \tilde{Y} , $\mathcal{T} = \emptyset$, n_{bqp} - maximum number of BQP inequalities to be added in one iteration.
while α is sufficiently large **do**
 Get an approximate maximizer of (17) by using L-BFGS-B method.
 Update R and \tilde{Y} according to (14) and (15).
 Remove inactive BQP inequalities from \mathcal{T} .
 Add the n_{bqp} most violated BQP inequalities for \tilde{Y} to \mathcal{T} .
 if the number of new violated inequalities added is below a threshold **then**
 Reduce α .
 end if
end while
Perform extra augmented Lagrangian iterations (with the previous α , without adding new cuts).
Compute $\tilde{Z} = W^\top (\tilde{L} - \mathcal{A}^\top \nu + \mathcal{B}^\top \mu - S)W$.
Use (18) with $\tilde{r} = \lfloor \frac{n}{2} \rfloor^2 + n$ to compute a valid lower bound LB.
output: LB

6 Numerical results

We implemented Algorithm 1 in Julia [3] version 1.10.0. For computing the basic DNN bound (DNN_{n+1}) we are using Mosek v10.2.3 [23] with the modeling language JuMP [21]. We use the Julia package LFBGSB v0.4.1 [24] as a wrapper to the L-BFGS-B solver. All computations were carried out on an AMD EPYC 7343 with 16 cores with 4.00 GHz and 1024GB RAM, operated under Debian GNU/Linux 11. The code is available at the arXiv page of this paper and at <https://github.com/melaniesi/CheegerConvexificationBounds.jl>.

The initial value of α is set to 1, and we stop reducing it once the penalty parameter α is smaller than 10^{-5} . We start to add violated cuts after the first five iterations. In each iteration, we then add the 500 most violated cuts, where we consider a BQP inequality to be violated if the violation is at least 10^{-3} . In case we find less than 50 new violated cuts, we reduce α by a factor of $\frac{3}{5}$. Cuts are removed from \mathcal{T} if the corresponding dual value is smaller than 10^{-5} . The cuts are added for the upper left $n \times n$ submatrix Y^{11} only. We perform at most 500 augmented Lagrangian iterations additionally at the end with constant α and stop as soon as the correction of the post processing is smaller than 0.01. We set the parameters of the L-BFGS-B solver to `maxiter=2000`, `factr=1e8`, and `m = 10`.

As benchmark instances, we use all instances already considered in [12] with less than 400 vertices and larger grlex and grevlex instances, cf. [11]. In [12] only grlex and grevlex instances with up to 92 vertices were considered, whereas we include all instances with fewer than 400 vertices. The benchmark set consists of graphs of random 0/1-polytopes, graphs of grlex and grevlex polytopes, instances from the 10th DIMACS challenge and some network instances. The edge expansion was computed in [12] for all instances considered therein. It was shown in [11] that the edge expansion of all grlex

instances is 1. Upper bounds, conjectured to be the edge expansion of the larger grevlex instances are taken from [25].

6.1 Comparing (DNN_{n+1}) with (DNN-P)

In Section 4.3 we proved that our new relaxation (DNN-P) is at least as good as the basic relaxation (DNN_{n+1}). We now compute these two bounds for several instances in order to show the significant dominance of our new relaxation. Table 1 is structured as follows. In the first three columns, we list the name of the instance, the number of vertices n , and the number of edges m . The edge expansion, or if not known, an upper bound on it, is reported in the fourth column UB of the table. In column 5 we report the lower bound (DNN_{n+1}) computed with Mosek, and in column 6 the relative gap of this lower bound to the upper bound. The relative gap is computed with the formula

$$\frac{\text{UB} - \text{LB}}{\text{UB}}, \quad (19)$$

where LB denotes a lower bound on the edge expansion, and UB denotes the upper bound on the edge expansion. In the last two columns of Table 1 we report the bound (DNN-P) approximated by Algorithm 1 without BQP inequalities and without the diagonal constraint (11) and its relative gap to the upper bound.

Note that all reported bounds are rounded to two decimal places.

Table 1 shows that except for the instance malariagenes-HVR1, the DNN relaxation (DNN-P) of dimension $2n + 3$ drastically reduces the relative gap to the upper bound compared to the basic DNN relaxation (DNN_{n+1}) of dimension $n + 1$. The relative gap of (DNN_{n+1}) is between 21% and 72% for all of our instances, with an average relative gap of 46.9%. The average relative gap of (DNN-P) is 8.6%. For 19 instances, the relative gap of (DNN-P) is at most 1%. Especially for most of the grlex instances, we were able to obtain a lower bound that is close to the optimum. For 9 instances, this bound rounded to two decimal places is equal to the rounded optimal values. Still, there are several benchmark instances with a relative gap of (DNN-P) being above 10%.

Table 1: Comparison of DNN relaxations without additional constraints.

	Instance			(DNN _{n+1})		(DNN-P)	
	n	m	UB	bound	gap (%)	bound	gap (%)
rand01-9-153-0	153	4081	18.75	14.33	23.6	17.75	5.3
rand01-9-153-1	153	4044	18.49	14.48	21.7	17.57	5.0
rand01-9-153-2	153	4107	19.00	14.26	25.0	17.83	6.2
rand01-8-164-0	164	1868	5.77	3.66	36.5	4.85	15.9
rand01-8-164-1	164	1837	5.35	3.28	38.8	4.68	12.5
rand01-8-164-2	164	1808	5.74	2.82	51.0	4.71	18.1
rand01-9-178-0	178	4590	17.08	13.33	22.0	16.07	5.9
rand01-9-178-1	178	4467	16.71	11.35	32.1	15.37	8.0
rand01-9-178-2	178	4537	16.75	10.67	36.3	15.64	6.7

Table 1 (cont.): Comparison of DNN relaxations without additional constraints.

	Instance			(DNN _{n+1})		(DNN-P)	
	n	m	UB	bound	gap (%)	bound	gap (%)
rand01-8-189-0	189	1768	4.22	2.61	38.2	3.46	18.2
rand01-8-189-1	189	1745	4.04	2.47	38.8	3.36	16.9
rand01-8-189-2	189	1719	4.06	2.28	43.8	3.33	17.9
rand01-9-203-0	203	4900	15.14	11.11	26.6	14.00	7.5
rand01-9-203-1	203	4781	14.84	9.87	33.5	13.54	8.8
rand01-9-203-2	203	4720	14.38	8.86	38.4	13.38	7.0
rand01-9-228-0	228	5065	13.24	8.94	32.4	12.02	9.2
rand01-9-228-1	228	4927	9.00	4.35	51.7	8.88	1.3
rand01-9-228-2	228	4984	12.82	7.12	44.5	11.77	8.2
rand01-9-253-0	253	5258	11.87	7.25	39.0	10.67	10.1
rand01-9-253-1	253	5053	9.00	4.34	51.8	8.89	1.2
rand01-9-253-2	253	5072	11.22	6.68	40.5	10.09	10.1
rand01-10-256-0	256	11056	30.48	20.20	33.7	29.38	3.6
rand01-10-256-1	256	10611	28.84	17.22	40.3	27.69	4.0
rand01-10-256-2	256	10746	29.38	22.28	24.1	28.13	4.2
rand01-9-278-0	278	5224	10.07	5.99	40.5	8.89	11.7
rand01-9-278-1	278	5007	9.00	4.14	54.0	8.05	10.6
rand01-9-278-2	278	5132	9.92	6.11	38.4	8.65	12.8
rand01-10-281-0	281	11828	28.90	20.21	30.1	27.71	4.1
rand01-10-281-1	281	11490	27.79	15.11	45.6	26.46	4.8
rand01-10-281-2	281	11454	27.75	19.31	30.4	26.44	4.7
grlex-7	29	119	1.00	0.51	49.3	0.98	1.7
grlex-8	37	176	1.00	0.47	53.0	1.00	0.1
grlex-9	46	249	1.00	0.43	56.6	1.00	0.2
grlex-10	56	340	1.00	0.41	58.5	1.00	0.5
grlex-11	67	451	1.00	0.41	59.5	0.99	0.9
grlex-12	79	584	1.00	0.39	60.8	0.99	0.8
grlex-13	92	741	1.00	0.38	62.3	0.99	1.0
grlex-14	106	924	1.00	0.37	63.2	1.00	0.3
grlex-15	121	1135	1.00	0.36	63.6	1.00	0.0
grlex-16	137	1376	1.00	0.36	64.3	0.99	0.9
grlex-17	154	1649	1.00	0.35	65.1	1.00	0.1
grlex-18	172	1956	1.00	0.34	65.6	0.99	0.8
grlex-19	191	2299	1.00	0.34	65.9	0.99	0.8
grlex-20	211	2680	1.00	0.34	66.3	0.98	1.8
grlex-21	232	3101	1.00	0.33	66.8	0.99	0.9
grlex-22	254	3564	1.00	0.33	67.1	1.00	0.0
grlex-23	277	4071	1.00	0.33	67.3	0.98	2.3

Table 1 (cont.): Comparison of DNN relaxations without additional constraints.

	Instance			(DNN _{n+1})		(DNN-P)	
	n	m	UB	bound	gap (%)	bound	gap (%)
grlex-24	301	4624	1.00	0.32	67.5	0.99	1.0
grlex-25	326	5225	1.00	0.32	67.9	0.94	5.9
grlex-26	352	5876	1.00	0.32	68.1	0.99	0.9
grlex-27	379	6579	1.00	0.32	68.2	0.96	3.7
grevlex-7	29	119	2.46	1.73	29.7	2.12	14.0
grevlex-8	37	176	2.83	1.90	33.0	2.35	17.2
grevlex-9	46	249	2.96	2.02	31.6	2.52	14.8
grevlex-10	56	340	3.22	2.21	31.6	2.77	14.1
grevlex-11	67	451	3.67	2.43	33.8	3.06	16.4
grevlex-12	79	584	3.92	2.61	33.4	3.31	15.7
grevlex-13	92	741	4.00	2.77	30.9	3.51	12.3
grevlex-14	106	924	4.47	2.95	33.9	3.76	16.0
grevlex-15	121	1135	4.83	3.17	34.4	4.03	16.6
grevlex-16	137	1376	4.99	3.36	32.6	4.28	14.1
grevlex-17	154	1649	5.27	3.53	33.0	4.49	14.7
grevlex-18	172	1956	5.67	3.72	34.4	4.75	16.3
grevlex-19	191	2299	5.94	3.93	33.7	5.02	15.5
grevlex-20	211	2680	6.06	4.13	31.9	5.26	13.2
grevlex-21	232	3101	6.53	4.30	34.1	5.50	15.7
grevlex-22	254	3564	6.83	4.49	34.3	5.74	16.0
grevlex-23	277	4071	6.99	4.70	32.7	6.02	13.9
grevlex-24	301	4624	7.35	4.90	33.4	6.16	16.3
grevlex-25	326	5225	7.72	5.08	34.3	6.28	18.7
grevlex-26	352	5876	7.94	5.27	33.7	6.27	21.0
grevlex-27	379	6579	8.13	5.48	32.6	6.55	19.4
karate	34	78	0.59	0.24	59.2	0.55	6.7
chesapeake	39	170	2.17	0.87	59.8	2.16	0.4
dolphins	62	159	0.29	0.09	69.4	0.29	0.1
lesmis	77	254	0.30	0.11	64.8	0.30	1.3
polbooks	105	441	0.37	0.18	50.0	0.31	14.9
adjnoun	112	425	1.00	0.37	62.9	0.99	0.9
football	115	613	1.07	0.76	29.3	0.97	9.4
jazz	198	2742	1.00	0.30	70.1	0.99	1.5
celegansneural	297	2148	1.00	0.43	56.7	0.92	8.2
moviegalaxies-567	52	146	0.38	0.18	52.7	0.38	1.1
moviegalaxies-52	59	119	0.54	0.18	65.7	0.43	19.2
terrorists-911	62	152	0.22	0.09	57.3	0.21	3.3

Table 1 (cont.): Comparison of DNN relaxations without additional constraints.

	Instance			(DNN _{n+1})		(DNN-P)	
	n	m	UB	bound	gap (%)	bound	gap (%)
train-terrorists	64	243	0.60	0.17	72.0	0.59	1.9
highschool	70	274	0.91	0.41	55.7	0.68	25.8
blumenau-drug	75	181	0.50	0.19	62.0	0.47	6.8
sp-office	92	9827	3.37	1.72	48.9	3.13	7.1
swingers	96	232	0.33	0.14	58.8	0.32	2.9
game-thrones	107	352	0.40	0.12	69.2	0.39	2.7
revolution	141	160	0.10	0.04	59.9	0.08	21.0
foodweb	183	2494	1.00	0.50	50.1	0.98	2.1
cintestinalis	205	2575	1.00	0.46	53.8	0.98	2.0
malariagenes-HVR1	307	2812	0.24	0.11	53.6	0.11	52.3

6.2 Detailed numerical tests of (DNN-PFRC)

In the following we now compare (DNN-P) to relaxation (DNN-PFRC) including additional scaled BQP inequalities, both computed approximately with our Algorithm 1. We omit instances from the table presenting computational results in this subsection where we could not get an improvement from our cutting planes. For several of these instances, the bound from (DNN-P) is already close to the optimal value, hence further improvement from cutting planes cannot be expected.

Table 2 is structured as follows. The first four columns describe the instance, i.e., the name of the instance, the number of vertices n , the number of edges m , and an upper bound UB on the edge expansion are given. In the next 3 columns, we report computational results for computing (DNN-P). Column 5 lists the lower bound on $h(G)$ obtained by Algorithm 1, in column 6 the number of edges m , and an upper bound UB on the edge expansion are given. In the next 3 columns, we report computational results for computing (DNN-PFRC). Column 5 lists the lower bound on $h(G)$ obtained by Algorithm 1, column 6 displays the relative gap (19), and in column 7 the wall-clock time in seconds needed to compute the lower bound is reported. The same numbers (bound, relative gap, computation time) for computing (DNN-PFRC) with Algorithm 1 are shown in the subsequent 3 columns. In the second to last column of the table, we report the number of cutting planes left in the last iteration of the algorithm, i.e., the number of cuts that were added and not removed by the algorithm. The total number of iterations needed by the algorithm to compute the DNN relaxation strengthened by scaled BQP cuts is given in the last column of the table.

Table 2 shows that for all graphs of random 0/1-polytopes, except 3 instances, the lower bound (DNN-PFRC) yields a relative gap below 1%. The computation time for all instances from graphs of random 0/1-polytopes was less than 49 minutes and 11.4 minutes on average. For the grlex instances, we were able to obtain for 5 further instances a lower bound that is, rounded to two decimal places, equal to the optimum by adding

cutting planes to the DNN relaxation. Considering the grevlex instances, there is only one instance where (DNN-PFRC) yields a relative gap below 1% compared to a relative gap of 12.3% from (DNN-P). Nevertheless, also for this class of benchmark instances, we were able to significantly reduce the relative gap to the upper bound/optimum by adding BQP inequalities, namely from an average of 15.8% to 4.4%. A similar observation can be made from the computational results on the DIMACS and network instances. In total, for 10 instances (DNN-PFRC) rounded to 2 decimal places closes the gap to the optimum $h(G)$.

Overall, our computational results demonstrate that in case the cutting planes improve the DNN relaxation of the edge expansion, the improvement is substantial. We were able to compute strong lower bounds on the edge expansion by computing (DNN-PFRC), a DNN of dimension up to 761×761 and up to 4272 cutting planes, with Algorithm 1 in less than 69 minutes.

Table 2: Computational results of Algorithm 1.

Instance	(DNN-P)			(DNN-PFRC)							
	n	m	UB	bound	gap (%)	time (s)	bound	gap (%)	time (s)	cuts	iterations
rand01-9-153-0	153	4081	18.75	17.75	5.3	67.0	18.67	0.4	136.6	1117	34
rand01-9-153-1	153	4044	18.49	17.57	5.0	68.9	18.43	0.3	105.9	907	30
rand01-9-153-2	153	4107	19.00	17.83	6.2	77.3	18.94	0.3	167.5	1406	63
rand01-8-164-0	164	1868	5.77	4.85	15.9	114.7	5.74	0.5	283.6	2073	78
rand01-8-164-1	164	1837	5.35	4.68	12.5	162.7	5.33	0.4	211.1	1510	56
rand01-8-164-2	164	1808	5.74	4.71	18.1	216.0	5.70	0.8	521.3	2782	57
rand01-9-178-0	178	4590	17.08	16.07	5.9	96.8	16.97	0.6	165.0	1978	43
rand01-9-178-1	178	4467	16.71	15.37	8.0	121.8	16.60	0.7	395.0	2174	70
rand01-9-178-2	178	4537	16.75	15.64	6.7	112.5	16.67	0.5	223.8	1737	62
rand01-8-189-0	189	1768	4.22	3.46	18.2	163.4	4.21	0.2	482.6	2278	48
rand01-8-189-1	189	1745	4.04	3.36	16.9	295.1	4.03	0.3	593.5	1963	91
rand01-8-189-2	189	1719	4.06	3.33	17.9	291.1	4.05	0.2	792.6	2723	73
rand01-9-203-0	203	4900	15.14	14.00	7.5	167.1	15.09	0.3	304.7	1787	100
rand01-9-203-1	203	4781	14.84	13.54	8.8	175.4	14.81	0.2	456.1	2133	51
rand01-9-203-2	203	4720	14.38	13.38	7.0	176.6	14.34	0.2	348.6	1770	50
rand01-9-228-0	228	5065	13.24	12.02	9.2	269.4	13.16	0.5	637.2	2491	41
rand01-9-228-1	228	4927	9.00	8.88	1.3	524.4	8.93	0.7	1111.7	2972	545
rand01-9-228-2	228	4984	12.82	11.77	8.2	505.3	12.74	0.6	529.4	1660	45
rand01-9-253-0	253	5258	11.87	10.67	10.1	797.6	11.77	0.8	1364.5	3234	61
rand01-9-253-1	253	5053	9.00	8.89	1.2	656.4	8.94	0.6	1283.1	3124	547
rand01-9-253-2	253	5072	11.22	10.09	10.1	536.6	11.18	0.4	915.9	2609	50
rand01-10-256-0	256	11056	30.48	29.38	3.6	302.0	30.24	0.8	486.6	1020	41
rand01-10-256-1	256	10611	28.84	27.69	4.0	775.0	28.82	0.1	719.0	2122	42
rand01-10-256-2	256	10746	29.38	28.13	4.2	318.6	29.17	0.7	469.5	2128	49
rand01-9-278-0	278	5224	10.07	8.89	11.7	878.5	9.79	2.8	760.7	2204	49
rand01-9-278-1	278	5007	9.00	8.05	10.6	1180.1	8.30	7.8	2922.7	4272	580

Table 2 (cont.): Computational results of Algorithm 1.

Instance	(DNN-P)			(DNN-PFRC)							
	n	m	UB	bound	gap (%)	time (s)	bound	gap (%)	time (s)	cuts	iterations
rand01-9-278-2	278	5132	9.92	8.65	12.8	763.3	9.76	1.6	1737.8	3091	61
rand01-10-281-0	281	11828	28.90	27.71	4.1	408.3	28.66	0.8	680.6	2068	52
rand01-10-281-1	281	11490	27.79	26.46	4.8	1103.3	27.66	0.5	858.7	2233	48
rand01-10-281-2	281	11454	27.75	26.44	4.7	418.1	27.54	0.8	693.2	1997	38
grlex-7	29	119	1.00	0.98	1.7	2.9	1.00	0.0	1.4	316	27
grlex-12	79	584	1.00	0.99	0.8	26.2	1.00	0.3	27.6	1423	47
grlex-13	92	741	1.00	0.99	1.0	43.2	1.00	0.3	47.6	885	60
grlex-16	137	1376	1.00	0.99	0.9	119.8	1.00	0.3	142.1	774	70
grlex-20	211	2680	1.00	0.98	1.8	575.5	0.99	1.1	570.3	974	526
grlex-23	277	4071	1.00	0.98	2.3	1415.0	0.99	1.2	1455.7	1278	527
grlex-24	301	4624	1.00	0.99	1.0	1542.0	1.00	0.0	1663.3	968	308
grlex-25	326	5225	1.00	0.94	5.9	2231.8	0.96	3.9	2250.9	443	525
grevlex-7	29	119	2.46	2.12	14.0	1.0	2.34	4.8	3.7	1613	40
grevlex-8	37	176	2.83	2.35	17.2	2.2	2.62	7.6	9.4	1843	48
grevlex-9	46	249	2.96	2.52	14.8	4.2	2.85	3.6	9.5	1449	50
grevlex-10	56	340	3.22	2.77	14.1	7.2	3.13	2.8	26.1	2136	66
grevlex-11	67	451	3.67	3.06	16.4	11.2	3.46	5.6	39.0	1488	93
grevlex-12	79	584	3.92	3.31	15.7	24.8	3.74	4.5	53.6	2151	73
grevlex-13	92	741	4.00	3.51	12.3	40.8	3.99	0.3	103.8	1652	77
grevlex-14	106	924	4.47	3.76	16.0	54.4	4.28	4.4	153.6	1488	98
grevlex-15	121	1135	4.83	4.03	16.6	80.5	4.59	5.0	172.7	1904	66
grevlex-16	137	1376	4.99	4.28	14.1	111.7	4.88	2.1	305.2	1250	369
grevlex-17	154	1649	5.27	4.49	14.7	163.2	5.13	2.5	330.8	2106	192
grevlex-18	172	1956	5.67	4.75	16.3	211.6	5.40	4.8	352.8	1533	150
grevlex-19	191	2299	5.94	5.02	15.5	267.5	5.71	3.8	529.0	1377	229

Table 2 (cont.): Computational results of Algorithm 1.

Instance	(DNN-P)			(DNN-PFRC)							
	n	m	UB	bound	gap (%)	time (s)	bound	gap (%)	time (s)	cuts	iterations
grevlex-20	211	2680	6.06	5.26	13.2	454.4	5.98	1.3	746.1	1183	242
grevlex-21	232	3101	6.53	5.50	15.7	585.1	6.23	4.6	772.6	1830	124
grevlex-22	254	3564	6.83	5.74	16.0	792.7	6.51	4.8	1134.0	2240	178
grevlex-23	277	4071	6.99	6.02	13.9	956.5	6.74	3.6	1310.9	1237	212
grevlex-24	301	4624	7.35	6.16	16.3	1836.0	6.70	8.9	1860.5	1558	544
grevlex-25	326	5225	7.72	6.28	18.7	2544.0	7.28	5.8	2984.0	2317	463
grevlex-26	352	5876	7.94	6.27	21.0	2169.6	7.51	5.5	4133.8	2373	557
grevlex-27	379	6579	8.13	6.55	19.4	2747.3	7.64	6.0	3515.5	1450	537
karate	34	78	0.59	0.55	6.7	5.5	0.59	0.0	5.2	518	28
polbooks	105	441	0.37	0.31	14.9	114.2	0.35	3.0	175.6	1033	40
football	115	613	1.07	0.97	9.4	86.4	1.07	0.0	118.1	382	28
celegansneural	297	2148	1.00	0.92	8.2	2595.9	0.96	3.6	3844.4	841	541
moviegalaxies-52	59	119	0.54	0.43	19.2	21.0	0.54	0.3	21.5	402	27
train-terrorists	64	243	0.60	0.59	1.9	46.7	0.60	0.1	24.6	293	28
highschool	70	274	0.91	0.68	25.8	33.4	0.90	1.7	52.4	1140	61
blumenau-drug	75	181	0.50	0.47	6.8	46.6	0.49	2.5	71.4	785	77
sp-office	92	9827	3.37	3.13	7.1	64.9	3.29	2.4	89.8	1333	50
game-thrones	107	352	0.40	0.39	2.7	127.3	0.40	0.4	108.5	279	32
revolution	141	160	0.10	0.08	21.0	242.2	0.09	7.9	233.7	1110	34
malariagenes-HVR1	307	2812	0.24	0.11	52.3	3225.4	0.23	4.4	2620.7	1608	477

7 Conclusion

This work demonstrates the effectiveness of the convexification technique by He, Liu, and Tawarmalani [13] in addressing the challenging problem of computing the edge expansion of a graph. By formulating the edge expansion as a completely positive program and introducing a doubly non-negative relaxation enhanced by cutting planes, we have developed a new approach for obtaining strong lower bounds. The augmented Lagrangian algorithm further improves the computational efficiency of solving this relaxation. Additionally, we provide a post processing routine to derive valid lower bounds. Numerical results show that our approach yields tight bounds and performs efficiently even for large graphs. For several instances, the rounded bound is equal to the optimal value or yields a very small relative gap. Some possible extensions of our approach would be to further strengthen the relaxation by adding McCormick inequalities.

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