Polyhedral Approximations of the Semidefinite Cone and Their Applications

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Abstract

Semidefinite optimization problems (SDPs) have a wide range of applications in convex optimization, combinatorial and nonconvex optimizations and control theory. The computational tractability of SDPs mainly comes from the fact that SDPs can be solved in polynomial time to any desired precision with interior-point methods. However, their computations become difficult when the size of the SDP becomes large. As an alternative class of methods to compensate for the weakness of interior-point methods, cutting-plane methods can obtain tightly approximated solutions of SDPs in a considerable amount of time. In this thesis, we focus on cutting-plane methods, which generate relaxations of SDPs and solve them as easily handled optimization problems. In particular, we focus on what impacts the initial relaxation problem, i.e., the approximations of the semidefinite cone.

We develop techniques to construct a series of sparse polyhedral approximations of the semidefinite cone. Motivated by the semidefinite (SD) bases proposed by Tanaka and Yoshise (2018), we propose a simple expansion of SD bases so as to keep the sparsity of the matrices composing it. We prove that the polyhedral approximation using our expanded SD bases contains the set of all diagonally dominant matrices, namely $\mathcal{DD}_n$, and is contained in the set of all scaled diagonally dominant matrices, namely $\mathcal{SDD}_n$. We also prove that $\mathcal{SDD}_n$ can be expressed using an infinite number of expanded SD bases.

We evaluate the dual cone of the set of diagonally dominant matrices (resp., scaled diagonally dominant matrices), namely $\mathcal{DD}_n^*$ (resp., $\mathcal{SDD}_n^*$), as an approximation of the semidefinite cone. Using the measure proposed by Blekherman et al. (2020) called the norm normalized distance, we prove that the norm normalized distance between a set $\mathcal{S}$ and the semidefinite cone has the same value whenever $\mathcal{SDD}_n^* \subseteq \mathcal{S} \subseteq \mathcal{DD}_n^*$. This implies that the norm normalized distance is not a sufficient measure to evaluate these approximations. As a new measure to compensate for the weakness of that distance, we propose a new measure, called the trace normalized distance. We prove that the trace normalized distance between $\mathcal{DD}_n^*$ and $\mathcal{S}_+^n$ has a different value from the one between $\mathcal{SDD}_n^*$ and $\mathcal{S}_+^n$, and give the exact values of these distances. We also present a new measure that calculates the minimum distance from some fixed points to a set. Using this measure, we show the tractability of our proposed approximation using expanded SD bases.

We use our approximation as the initial approximation in the cutting-plane method for solving doubly nonnegative optimization problems and a semidefinite relaxation of the maximum stable set problem. It is found that for large-scale instances, the proposed method with expanded SD bases is significantly more efficient than methods using other existing approximations or solving the semidefinite optimization problem directly.

Keywords: Semidefinite optimization problem; Polyhedral approximation; Factor width; Diagonally dominant matrix; Scaled diagonally dominant matrix; Expanded semidefinite basis; Norm normalized distance; Trace normalized distance; Cutting-plane method.

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Notation

Sets

$\mathbb{R}$	Space of real numbers
$\mathbb{N}$	Set of nonnegative integers
$\mathbb{R}^n$	Space of real n-dimensional vectors ($n \times 1$ matrices)
$\mathbb{R}^{n\times m}$	Space of real $n \times m$ matrices
$\mathbb{S}^n$	Space of real $n \times n$ symmetric matrices
$\mathcal{N}^n$	Set of real $n \times n$ nonnegative symmetric matrices
$\mathcal{S}_+^n$	Set of real $n \times n$ positive semidefinite matrices
$\mathcal{S}_+^n \cap \mathcal{N}^n$	Doubly NonNegative (DNN) cone
$\mathcal{S}_+^n + \mathcal{N}^n$	Minkowski sum of $\mathcal{S}_+^n$ and $\mathcal{N}^n$
$\mathcal{C}_n$	Copositive cone
$\mathcal{O}^n$	Set of $n \times n$ orthogonal matrices
$\mathcal{K}^*$	Dual cone of a cone $\mathcal{K} \subseteq \mathbb{S}^n$

Vectors and matrices

I	Identity matrix
e_i	Vector with a 1 at the ith coordinate and 0 elsewhere
X^T	Transpose of matrix X
$\mathrm{Tr}(X)$	Trace of matrix X
$\langle X, Y\rangle$	Trace inner product of matrices X and Y
$\|X\|_F$	Frobenius norm of matrix X
$\lambda_{\min}(X)$	Smallest eigenvalue of matrix X

Acronyms

LP	Linear optimization problem
SOCP	Second order cone optimization problem
SDP	Semidefinite optimization problem
DNN	Doubly nonnegative
CP	Copositive optimization problem

Chapter 1

Introduction

1.1 Linear optimization and semidefinite optimization

An optimization problem is a problem that minimizes or maximizes an objective function under some constraints. Optimization problems arise in many fields, such as transportation, economies, control engineering, management science. Based on whether the variables are continuous or discrete, optimization problems can be classified into two types: discrete optimization problems and continuous optimization problems. One major subfield in continuous optimization is convex optimization, which considers when the objective function and the set of feasible solutions are both convex. A basic and well-known class of convex optimization problems is the class of linear optimization problems, where the objective function and all constraints are linear.

Linear optimization problems

A linear optimization problem (LP) in standard form is written as

$$\begin{aligned} \min\ & \langle c, x\rangle \\ \text{s.t. } & \langle a_j, x\rangle = b_j, j = 1, 2, \dots, m, \\ & x \in \mathbb{R}^n_+, \end{aligned}$$

where $c, a_j \in \mathbb{R}^n$, $b_j \in \mathbb{R}$ $(j = 1, \dots, m)$, $\mathbb{R}^n_+$ is the set of entrywise nonnegative vectors, and $\langle x, y\rangle := x^T y$ is the inner product over $\mathbb{R}^n$.

In 1947, Dantzig [33] formulated linear optimization problems and discovered the simplex method for solving them. Although the simplex method is efficient in practice, the worst-case complexity of the simplex method with Dantzig's most-negative-reduced-cost pivot rule is known to be exponential time through an example by Klee and Minty [69]. Khachiyan [66] was the first to show that LPs are polynomial-time solvable by using the ellipsoid method, though its performance in practice was not promising (e.g., [19]). In 1984, Karmarkar [64] proposed a new polynomial-time algorithm, called the interior-point method, which is efficient in practice. Karmarkar's method encourages a large number of studies on interior-point methods (for more details, see e.g., [50, 107]). Based on the study of Megiddo [85], Kojima, Mizuno and Yoshise [71] developed a primal-dual interior point method, which generates a sequence of primal and dual interior solutions of an LP. As a powerful class of interior-point methods, primal-dual methods have been studied by many researchers since 1986 (e.g., [87] and [84]). The recent widely used LP solvers (e.g., Gurobi [53] and CPLEX [32]) often implement simplex methods and primal-dual interior point methods. For a more detailed survey of algorithms for LPs, we refer interested readers to [109] and [119]. It is worth noting that in 2015, Chubanov [31] proposed another polynomial-time algorithm for solving linear feasibility problems, which leads to a new stream of researches (e.g., [100]).

Linear optimization problems can be seen as special cases of semidefinite optimization problems, which have gained increasing attention since the 1990s. The tractability of semidefinite optimization problems comes from the fact that they have a wild range of applications in convex optimizations, combinatorial and nonconvex optimizations and control theory. More importantly, semidefinite optimization problems can be solved in polynomial time to any desired precision with interior-point methods (e.g., [3]). Next, we look into semidefinite optimization problems and introduce some of their applications and algorithms.

Semidefinite optimization problems

A semidefinite optimization problem (SDP) is an optimization problem in variables in the space of real symmetric matrices with a linear objective function and linear constraints over the semidefinite cone. We denote the space of symmetric matrices as $\mathbb{S}^n := \{X \in \mathbb{R}^{n\times n} \mid X_{i,j} = X_{j,i}\ (1 \leq i < j \leq n)\}$ and the semidefinite cone as $\mathcal{S}^n_+ := \{X \in \mathbb{S}^n \mid d^T X d \geq 0 \text{ for any } d \in \mathbb{R}^n\}$. Accordingly, we can readily define an SDP in the standard form, as

$$\begin{aligned} \min\ & \langle C, X\rangle \\ \text{s.t. } & \langle A_j, X\rangle = b_j, j = 1, 2, \ldots, m, \\ & X \in \mathcal{S}^n_+, \end{aligned} \tag{1.1}$$

where $C \in \mathbb{S}^n$, $A_j \in \mathbb{S}^n$, $b_j \in \mathbb{R}$ $(j = 1, 2, \ldots, m)$, and $\langle A, B\rangle := \mathrm{Tr}(A^T B) = \sum_{i,j=1}^n A_{i,j}B_{i,j}$ is the inner product over $\mathbb{S}^n$.

Semidefinite optimization has wide applications in convex optimization, such as convex quadratically constrained optimization and eigenvalue optimization (e.g., [36, 56]). As a special class of convex optimization, semidefinite optimization is also a powerful tool that provides convex relaxations for combinatorial and nonconvex optimizations, such as the max-cut problem (e.g., [28, 48]) , the k-equipartition problem (e.g., [63, 118]) and the quadratic knapsack problem (e.g.[57, 58]). Some of these relaxations can even attain the optimum, as shown in [67] and [77]. There are also many applications of SDPs in control theory, see e.g., [25, 92]. Interested readers may find more details about SDPs and their applications in [4, 55, 79, 108, 111, 112, 118]. Here, we briefly introduce two applications of semidefinite optimization in convex and combinatorial optimizations.

Example 1: Convex quadratically constrained quadratic optimization

First, we present an application of semidefinite optimization in convex optimization. Consider a quadratically constrained quadratic optimization problem (QCQP) of the form:

$$\begin{aligned} (\text{QCQP}): \min_{x\in\mathbb{R}^n} \quad & x^T Q_0 x + d_0^T x + e_0 \\ \text{s.t.} \quad & x^T Q_i x + d_i^T x + e_i \leq 0,\ i = 1, \ldots, m, \end{aligned}$$

where $Q_i \in \mathcal{S}_+^n,\ d_i \in \mathbb{R}^n$ and $e_i \in \mathbb{R}$, $i = 0, \ldots, m$. This problem is equivalent to

$$\begin{aligned} (\text{QCQP}): \min_{x\in\mathbb{R}^n,\alpha\in\mathbb{R}} \quad & \alpha \\ \text{s.t.} \quad & x^T Q_0 x + d_0^T x + e_0 \leq \alpha \\ & x^T Q_i x + d_i^T x + e_i \leq 0,\ i = 1, \ldots, m. \end{aligned}$$

For each semidefinite matrix $Q_i \in \mathcal{S}_+^n$ where $i = 0, \ldots, m$, we know that there exists a positive integer k_i and a matrix $M_i \in \mathbb{R}^{k_i \times n}$ such that $Q_i = M_i^T M_i$. A fundamental property of semidefinite matrices (see, e.g., Fact 11. [108]) states that with matrices $C \in \mathbb{S}^{n_2}, B \in \mathbb{R}^{n_1 \times n_2}$ and $A \in \mathbb{S}^{n_1}$ positive definite (i.e., $\forall d \in \mathbb{R}^{n_1} \setminus \{0\}, d^T A d > 0$), we have

$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \in \mathcal{S}_+^{n_1+n_2} \text{ if and only if } C - B^T A^{-1} B \in \mathcal{S}_+^{n_2}.$$

As its direct corollary, one can easily see that the problem (QCQP) can be equivalently written as the following SDP:

$$
\begin{aligned}
\min_{x\in\mathbb{R}^n,\alpha\in\mathbb{R}} \quad & \alpha \\
\text{s.t.} \quad & \begin{pmatrix} I_{k_0} & M_0x \\ (M_0x)^T & -e_0 - d_0^T x + \alpha \end{pmatrix} \in \mathcal{S}_+^{k_0+1} \\
& \begin{pmatrix} I_{k_i} & M_ix \\ (M_ix)^T & -e_i - d_i^T x \end{pmatrix} \in \mathcal{S}_+^{k_i+1}, \ i = 1, \dots, m,
\end{aligned}
$$

where I_{k_i} is the $k_i \times k_i$ identity matrix.

Example 2: The max-cut problem

Next, we introduce an application of semidefinite optimization in combinatorial optimization. Consider an undirected graph with a set of nodes $\mathcal{N} = \{1, \dots, n\}$ and a set of edges $\mathcal{E}$. Let $w_{i,j} = w_{j,i} \geq 0$ be the weight on each edge $(i,j) \in \mathcal{E}$. For a subset of nodes $\mathcal{K} \subseteq \mathcal{N}$, let $\delta(\mathcal{K}) := \{(i,j) \in \mathcal{E} \mid i \in \mathcal{K}, j \notin \mathcal{K}\}$, called the cut determined by $\mathcal{K}$. The max-cut problem is to find a cut of maximum weight, i.e., find a subset of nodes $\mathcal{K} \subseteq \mathcal{N}$, such that $\sum_{(i,j)\in\delta(\mathcal{K})} w_{i,j}$ attains its maximum. We assume that the graph is complete (i.e., each pair of nodes are adjacent) by setting $w_{i,j} = 0$ for $(i,j) \notin \mathcal{E}$. We also let $w_{i,i} = 0$ for $i = 1, \dots, n$. Then the max-cut problem can be formulated as

$$
\begin{aligned}
\text{(MAXCUT)} \ \max \quad & \frac{1}{4}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}(1 - x_i x_j) \\
\text{s.t.} \quad & x_i \in \{1, -1\}, i = 1 \dots, n.
\end{aligned}
$$

Let W be a matrix where $W_{i,j} = -\frac{w_{i,j}}{4}$ for $i \neq j$ and $W_{i,i} = \sum_{j=1}^{n} \frac{w_{i,j}}{4}$ for $i = 1, \dots, n$. By setting $X = xx^T$, (MAXCUT) can be equivalently formulated as

$$
\begin{aligned}
\text{(MAXCUT)} \ \max \quad & \langle W, X \rangle \\
\text{s.t.} \quad & X_{i,i} = 1, i = 1 \dots, n, \\
& X = xx^T.
\end{aligned}
$$

Note that $X = xx^T$ if and only if $X \in \mathcal{S}_+^n$ and $\text{rank}(X) = 1$. Therefore, we can obtain a relaxed semidefinite optimization problem by removing the rank constraint:

$$\begin{aligned} \text{(reSDP)} \quad \max \quad & \langle W, X \rangle \\ \text{s.t.} \quad & X_{i,i} = 1, i = 1 \ldots, n, \\ & X \in \mathcal{S}_+^n. \end{aligned}$$

Let OPT be the optimal value of (MAXCUT). Goemans and Williamson [48] used (reSDP) to derive a randomized algorithm, which produces a cut whose expected objective value is at least $0.87856 OPT$.

1.2 Algorithms for solving SDPs

An important difference between semidefinite optimization and linear optimization is that there is no straightforward or practical simplex method for SDPs (c.f. [111]). The ellipsoid method of Yudin and Nemirovsky [122] and Shor [104] can be used to solve SDPs, but it is slow in practice. The computational tractability of semidefinite optimization problems mainly comes from the fact that SDPs can be solved in polynomial time to any desired precision with interior-point methods. Nesterov and Nemirovski [90] showed that interior-point methods for linear optimization can be generalized to convex optimization. Independently, Alizadeh [3] generalized interior-point methods from linear optimization to semidefinite optimization. In recent years, state-of-the-art SDP solvers implementing interior-point methods have been developed, such as SDPA [120], SeDuMi [105], SDPT3 [110], and Mosek [6]. However, their computations become difficult when the size of the SDP becomes large. For example, Mosek Optimizer 9.0 cannot solve an instance of Problem (1.1) with $n = 300$ and entry-wise nonnegative constraints within 20000s on a Windows PC with an Intel(R) Core(TM) i7-6700 CPU running at 3.4 GHz and 16 GB of RAM. This deficiency is mainly due to the memory requirements of interior-point methods, i.e., their iterations generate points in the interior feasible set of an SDP and require storage and computations on large dense matrices.

To compensate for the weakness of interior-point methods, many researchers have developed techniques and alternative algorithms for solving structured and general large-scale SDPs.

Many techniques have been developed for SDPs with special structures. For large-scale SDPs with special symmetric or facial structures, one may use preprocessing techniques to reduce the size of the SDPs, which leads to facial reduction methods (e.g., [24, 94, 95, 113, 125]) and symmetry reduction methods (e.g., [37, 60, 96, 101]). For SDPs with chordal sparsity structures, one can transform a large semidefinite constraint into a set of lower-dimensional semidefinite constraints with equality constraints [52, 61]. Interior-point methods (e.g., [46, 5]) and first-order methods (e.g., [82, 123]) for solving SDPs with chordal sparsity structures are developed. For SDPs in low-rank approximation problems (e.g., in matrix completion problems), which expect to find low-rank solutions with reasonable objective values, one may consider dealing with problems only in lower dimensions and increase computational efficiency. This idea inspired algorithms for solving SDPs with low-rank structures such as the Burer-Monteiro method (e.g., [29, 30]) and the Frank-Wolfe based methods (e.g., [45, 54]).

There are other methods for solving general large-scale SDPs. For example, an alternative for solving large-scale SDPs is to use first-order methods, which is simpler than second-order interior-point methods but may result in less accurate solutions (i.e., small violations on constraints may occur). This encourages some researches on the alternating direction method of multipliers (ADMM) for solving SDPs (e.g., [62, 91, 116]).

Another idea is to generate relaxations of SDPs and solve them as easily handled optimization problems, e.g., LPs and second-order cone optimization problems (SOCPs), which leads to cutting-plane methods (e.g., [1, 2, 72, 73, 75, 114]). Since the relaxed problems, i.e., LPs and SOCPs, can be solved significantly faster than SDPs by using powerful LP and SOCP solvers, the cutting-plane methods allow us to sacrifice solution optimality for computational efficiency.

Note that there are many other alternatives to interior-point methods for SDPs, such as the accelerated first-order method by Renegar [98] and the generalizations of the Chubanov's algorithm (e.g., [80, 93]). We refer interested readers to a recent survey on alternative methods for solving large-scale SDPs by Majumdar, Hall and Ahmadi [83].

In practice, when considering a semidefinite optimization problem, sometimes we only need to obtain a lower bound of the optimal value of the SDP instead of solving it to the optimum. The cutting-plane methods can be used to provide tight bounds on the optimal value of an SDP within a reasonable time. This merit encourages us to gain insight into the cutting-plane methods.

Cutting-plane methods for solving SDPs

The cutting-plane method was first used on the traveling salesman problem by Dantzig, Fulkerson, and Johnson [34, 35] in 1954. It was used in 1958 by Gomory [49] to solve integer linear programming problems. In 1960, Kelly [65] proposed a cutting-plane method for solving convex optimization problems. As SDPs became popular, cutting-plane methods came to be used on them as well; see, for instance, Krishnan and Mitchell [73, 74, 75] and

Konno et al. [72]. Kobayashi and Takano [70] applied it to a class of mixed-integer SDPs. In [1], Ahmadi, Dash, and Hall applied it to nonconvex polynomial optimization problems and copositive optimization problems.

The cutting-plane method solves an SDP by transforming it into a relaxed optimization problem (e.g., an LP or an SOCP), adding cutting-planes at each iteration to cut the current approximate solution out of the feasible region in the subsequent iterations, and get close to the optimal value. There are two essential questions about the cutting-plane method for solving SDPs:

Q1 How to add cutting-planes to the relaxed problem?

Q2 How to obtain an initial relaxation problem from a given SDP?

As for the first question, one common strategy for generating cuts at each iteration is to obtain the eigenvector $d \in \mathbb{R}^n$ corresponding to the least eigenvalue of the current solution $\hat{X}$. Then, dd^T either verifies $\hat{X} \in \mathcal{S}^n_+$ if $\langle dd^T, \hat{X} \rangle \geq 0$, or generates a separating hyperplane such that $\langle dd^T, \hat{X} \rangle < 0$ and $\langle dd^T, X \rangle \geq 0$ for all $X \in \mathcal{S}^n_+$. Note that there are other kinds of cuts. Bertsimas and Cory-Wright [17] proposed the nuclear norm cut, which penalizes the sum of absolute values of all eigenvalues instead of the least eigenvalue of the current solution. The eigenvector cuts and the nuclear norm cuts are LP-based cuts because they involve only linear constraints. Ahmadi et al. [1] introduced an SOCP-based cut, which ensures that the 2×2 matrix $(p_1, p_2)^T X (p_1, p_2)$ is semidefinite, where p_1, p_2 are eigenvectors corresponding to the 2 least eigenvalues of the current solution.

As in the second question, the choice of the initial relaxation problem, is also an important issue. If the initial relaxation problem has a better lower bound on the optimal value, then we may need less effort to get close to the optimum. If the initial relaxation problem is easier to handle, then the algorithm may be more computationally efficient. These observations inspired us to focus on what impacts the initial relaxation problem.

In the above-mentioned cutting-plane methods for SDPs, the semidefinite constraint $X \in \mathcal{S}^n_+$ in (1.1) is first relaxed to $X \in \mathcal{K}_{\text{out}}$, where $\mathcal{S}^n_+ \subseteq \mathcal{K}_{\text{out}} \subseteq \mathbb{S}^n$. We call such a set $\mathcal{K}_{\text{out}}$ an initial outer approximation of $\mathcal{S}^n_+$, and the relaxed problem with constraint $X \in \mathcal{K}_{\text{out}}$ is an initial relaxation of the SDP. If $\mathcal{K}_{\text{out}}$ is given by linear constraints, then the initial relaxation gives an LP and can be solved by powerful LP solvers; if $\mathcal{K}_{\text{out}}$ is given by second-order constraints, then the initial relaxation becomes an SOCP. To improve the performance of these cutting-plane methods, we consider generating initial relaxations for SDPs that are both tight and computationally efficient and focus on approximations of $\mathcal{S}^n_+$.

1.3 Polyhedral approximations of the semidefinite cone

Many approximations of $\mathcal{S}^n_+$ have been proposed on the basis of its well-known properties. Kobayashi and Takano [70] used the fact that the diagonal elements of semidefinite matrices are nonnegative. Konno et al. [72] imposed an assumption that all diagonal elements of the variable X in the SDPs appearing in their iterative algorithm are bounded by a constant. The sets of diagonally dominant matrices, namely $\mathcal{DD}_n$, and the set of scaled diagonally dominant matrices, namely $\mathcal{SDD}_n$, are known to be cones contained in $\mathcal{S}^n_+$, (see, e.g., [59] and [1] for details). The inclusive relation among them has been studied in, e.g., [12] and [18]. Ahmadi et al. [1] used these sets as initial approximations of their cutting-plane method. Boman et al. [23] defined the factor width of a semidefinite matrix, and Permenter and Parrilo used it to generate approximations of $\mathcal{S}^n_+$, which they applied to facial reduction methods in [95].

Among these approximations, we focus on those approximations given by the intersection of a finite number of closed half-spaces, i.e., the polyhedral approximations. Relaxations with polyhedral approximations can be solved efficiently and accurately by state-of-the-art LP solvers, e.g., Gurobi [53].

Tanaka and Yoshise defined various bases of $\mathbb{S}^n$, wherein each basis consists of $\frac{n(n+1)}{2}$ semidefinite matrices, called semidefinite (SD) bases, and used them to devise polyhedral approximations of $\mathcal{S}^n_+$ [106]. They showed that the conical hull of SD bases and its dual cone give inner and outer polyhedral approximations of $\mathcal{S}^n_+$, respectively. In this thesis, we focus on the fact that SD bases are sometimes sparse, i.e., the number of nonzero elements in a matrix is relatively small, and hence, it is not so computationally expensive to solve polyhedrally approximated problems in such SD bases. We call such an approximation a *sparse polyhedral approximation*.

The research by Tanaka and Yoshise [106] motivated us to construct tighter and sparse polyhedral approximations of $\mathcal{S}^n_+$ by using SD bases in order to solve complicated large-scale SDPs, e.g., the doubly nonnegative (DNN) relaxations of copositive optimization problems.

Evaluating the approximations of the semidefinite cone

Although the inclusive relationship of the approximations as mentioned above has been given (e.g., [2], [17], [114]), theoretical analyses of how well these sets approximate the semidefinite cone have been limited.

Fawzi [43] evaluated how polytopes can approximate a compact slice of the semidefinite cone by using a measure called extension complexity. Bertsimas and Cory-Wright [17] evaluated the dual cones of $\mathcal{DD}_n$ and $\mathcal{SDD}_n$ as approximations of the semidefinite cone by comparing lower bounds of the minimum eigenvalues of matrices from these two sets.

Blekherman et al. [20] proposed an evaluation method called the norm normalized distance. The norm normalized distance between a given approximation $\mathcal{S} \subseteq \mathbb{S}^n$ and $\mathcal{S}^n_+$ is the maximum distance from a matrix $X \in \mathcal{S}$ to $\mathcal{S}^n_+$, where the Frobenius norm of the matrix X is assumed to be one. Using this measure, they evaluated the set of matrices whose 2×2 principal submatrices are positive semidefinite, namely $\mathcal{S}^{n,k}$, as an approximation of the semidefinite cone. They obtained several upper bounds and lower bounds of the norm normalized distance between $\mathcal{S}^{n,k}$ and $\mathcal{S}^n_+$.

Motivated by these results, we conduct theoretical analyses and evaluate the approximations of the semidefinite cone, including $\mathcal{DD}_n$, $\mathcal{SDD}_n$ and the polyhedral approximation we proposed.

1.4 Contribution and outline

The contributions of this paper are summarized as follows.

- In this thesis, we propose a simple expansion of SD bases without losing the sparsity of the matrices and prove that one can generate a sparse polyhedral approximation of $\mathcal{S}^n_+$ that contains the set of diagonally dominant matrices and is contained in the set of scaled diagonally dominant matrices.

- We show that the norm normalized distance between a set $\mathcal{S}$ and $\mathcal{S}^n_+$ has the same value whenever $\mathcal{SDD}^*_n \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$. This implies that the norm normalized distance is not a sufficient measure to evaluate these approximations. As a new measure to compensate for the weakness of that distance, we introduce a new distance, called the trace normalized distance. We prove that the trace normalized distance between $\mathcal{DD}^*_n$ and $\mathcal{S}^n_+$ has a different value from the one between $\mathcal{SDD}^*_n$ and $\mathcal{S}^n_+$, and give the exact values of these distances. We also present a new measure that calculates the minimum distance from some fixed points to a set. Using this measure, we show the tractability of our proposed approximation using expanded SD bases.

- The expanded SD bases are used by cutting-plane methods for solving random doubly nonnegative optimization problems and a semidefinite relaxation of the maximum stable set problem. It is found that the proposed method with expanded SD bases are significantly more efficient than methods using other approximations or solving the semidefinite relaxation problem directly.

The organization of this thesis is as follows. Chapter 2 covers some preliminaries on convex analysis and conic optimization problems. In Chapter 3, various approximations of $\mathcal{S}^n_+$ are introduced, including those based on the factor width by Boman et al. [23], diagonal dominance by Ahmadi et al. [1], and SD bases by Tanaka and Yoshise [106]. An expansion of SD bases and an analysis of its theoretical properties are also provided. In Chapter 4, the norm normalized distance and the proposed trace normalized distance are used to measure the above approximations. In Chapter 5, we introduce the cutting-plane method with different approximations of $\mathcal{S}^n_+$ for calculating lower bounds of random DNN problems and upper bounds of the maximum stable set problem. We also describe the results of numerical experiments and evaluate the efficiency of our proposed method with expanded SD bases. Note that the contents in Chapter 3 and 5 are based on the published study [114] and the contents in Chapter 4 are based on the recent paper [115].

Chapter 2

Preliminaries

In this chapter, we will first cover some preliminaries on convex analysis, focusing on convex cones, especially polyhedral cones and the semidefinite cone. The properties of cones play a fundamental role in this thesis. We next present some basic results on conic optimization problems. For more detailed contents, we refer interested readers to some common reference on convex analysis [16, 26, 99], and on semidefinite and conic optimizations [22, 118].

2.1 Convex analysis

Let $\mathbb{R}^n$ be the n-dimensional real vector space, equipped with the inner product of two vectors $x, y \in \mathbb{R}^n$: $\langle x, y\rangle = x^T y = \sum_{i=1}^n x_i y_i$. The associated norm on $\mathbb{R}^n$ is $\|x\|_2 = \sqrt{\langle x, x\rangle} = \sqrt{\sum_{i=1}^n x_i^2}$, called the Euclidean norm (or l_2-norm). We first give the definition and some properties of convex cones.

2.1.1 Convex cones

A set $\mathcal{C} \subseteq \mathbb{R}^n$ is called a convex set if for any pair of points $x, y \in \mathcal{C}$ and $0 \leq \lambda \leq 1$,

$$(1-\lambda)x + \lambda y \in \mathcal{C}.$$

It is well-known that if $\mathcal{C}_1$ and $\mathcal{C}_2$ are convex sets, then $\mathcal{C}_1 \cap \mathcal{C}_2$ is also convex.

We then give the definition of extreme points of a convex set (see, e.g. [15]). Given a convex set $\mathcal{C} \subseteq \mathbb{R}^n$, a point $x \in \mathcal{C}$ is called an extreme point of $\mathcal{C}$ if there do not exist points $y, z \in \mathcal{C}$ where $y \neq x$ and $z \neq x$, and a scalar $\alpha \in (0,1)$ such that $x = \alpha y + (1-\alpha)z$.

Let $\mathcal{C} \subseteq \mathbb{R}^n$ be a convex set. A function $f : \mathcal{C} \to \mathbb{R}$ is a convex function if for any pair of points $x, y \in \mathcal{C}$ and $0 \leq \lambda \leq 1$,

$$f((1-\lambda)x + \lambda y) \leq (1-\lambda)f(x) + \lambda f(y).$$

The Bauer maximum principle [11] (see also, [76]) states that any continuous convex function defined on a compact (i.e., closed and bounded) convex set in $\mathbb{R}^n$ attains its maximum at some extreme point of the set.

An essential fact about convex sets is that one can project any point onto a closed convex set by taking the closest point in the set.

Lemma 2.1.1. (*Proposition 2.2.1 (a), (c) [16]*) Let $\mathcal{C} \subseteq \mathbb{R}^n$ be a nonempty closed convex set. Let $x \in \mathbb{R}^n \setminus \mathcal{C}$ be a point outside $\mathcal{C}$. Then there exists a unique point $P_{\mathcal{C}}(x)$ in $\mathcal{C}$ which is closest to x:

$$P_{\mathcal{C}}(x) := \text{argmin}_{y \in \mathcal{C}} \|x - y\|_2.$$

$P_{\mathcal{C}}(x)$ is called the projection of x on $\mathcal{C}$. Moreover, the map $P_{\mathcal{C}} : \mathbb{R}^n \to \mathcal{C}$ is continuous and nonexpansive, i.e., for any two points $x, y \in \mathbb{R}^n$,

$$\|P_{\mathcal{C}}(x) - P_{\mathcal{C}}(y)\|_2 \leq \|x - y\|_2.$$

With the above lemma and Proposition 2.2.1 (d) [16], we know that the following lemma holds.

Lemma 2.1.2. Let $P_{\mathcal{C}}(x)$ be the projection of $x \in \mathbb{R}^n$ on a closed convex set $\mathcal{C} \subseteq \mathbb{R}^n$. Then the distance function $f(x) := \|x - P_{\mathcal{C}}(x)\|_2$ is continuous and convex on $\mathbb{R}^n$.

Next we introduce the definition of cones. A set $\mathcal{K} \subseteq \mathbb{R}^n$ is a cone if it is closed under nonnegative scaling, i.e., for any point $x \in \mathcal{K}$ and scalar $\alpha \geq 0$,

$$\alpha x \in \mathcal{K}.$$

We call a cone $\mathcal{K} \subset \mathbb{R}^n$ proper if it has a nonempty interior and is closed, pointed (i.e., $\mathcal{K} \cap -\mathcal{K} = \{0\}$), and convex. For example, the nonnegative orthant $\mathbb{R}^n_+$ is a proper cone.

The dual cone of a cone $\mathcal{K} \subseteq \mathbb{R}^n$ is defined as

$$\mathcal{K}^* := \{x \in \mathbb{R}^n \mid \forall y \in \mathcal{K}, \langle x, y \rangle \geq 0\}.$$

The set $\mathcal{K}^*$ is a closed and convex cone. Also, if two cones satisfy $\mathcal{K}_2 \subseteq \mathcal{K}_1$, then we have $\mathcal{K}_1^* \subseteq \mathcal{K}_2^*$. A convex cone $\mathcal{K}$ is called self-dual if $\mathcal{K} = \mathcal{K}^*$. For example, $\mathbb{R}^n_+$ is self-dual.

The conical hull of a set $\mathcal{A} \subseteq \mathbb{R}^n$ is defined as

$$\operatorname{cone}(\mathcal{A}) := \{\sum_{i=1}^{k} \alpha_i x_i \mid k \in \mathbb{N}, \alpha_1, \ldots, \alpha_k \geq 0, x_1, \ldots, x_k \in \mathcal{A}\},$$

where $\mathbb{N}$ is the set of nonnegative integers. It is straightforward that if $\mathcal{A} \subseteq \mathcal{B}$, then $\operatorname{cone}(\mathcal{A}) \subseteq \operatorname{cone}(\mathcal{B})$.

2.1.2 Polyhedral cones and polyhedra

Polyhedral cones are special cases of convex cones, and are closely related to linear optimization problems. A convex cone $\mathcal{K} \subseteq \mathbb{R}^n$ is called polyhedral if

$$\mathcal{K} = \{x \in \mathbb{R}^n \mid \langle a_j, x \rangle \leq 0, j = 1, \ldots, m\}$$

for a positive integer m and some $a_1, \ldots, a_m \in \mathbb{R}^n$.

A convex cone $\mathcal{K} \subseteq \mathbb{R}^n$ is called finitely generated if

$$\mathcal{K} = \operatorname{cone}(\mathcal{A})$$

for some finite set $\mathcal{A} \subseteq \mathbb{R}^n$. The following fundamental theorem of polyhedral cones follows from the results of Minkowski [86] and Weyl [117].

Theorem 2.1.3. *(Minkowski-Weyl theorem, see Corollary 7.1a in [102])* A convex cone is polyhedral if and only if it is finitely generated.

A set $\mathcal{P} \subseteq \mathbb{R}^n$ is called a polyhedron if

$$\mathcal{P} = \{x \in \mathbb{R}^n \mid \langle a_j, x \rangle \leq b_j, j = 1, \ldots, m\}$$

for some $a_1, \ldots, a_m \in \mathbb{R}^n$, $b_1, \ldots, b_m \in \mathbb{R}$ and a positive integer m. One can see that polyhedral cones are special cases of polyhedra with $b_1, \ldots, b_m = 0$. Next we give a well-known characterization of extreme points of a polyhedron.

Lemma 2.1.4. (*see, e.g., Proposition 2.1.4 (a) [15], Theorem 5.7 [103]*) Let $\mathcal{P}$ be a polyhedron in $\mathbb{R}^n$:

$$\mathcal{P} = \{x \in \mathbb{R}^n \mid \langle a_j, x \rangle \leq b_j, j = 1, \ldots, m\}$$

for some $a_1, \ldots, a_m \in \mathbb{R}^n$, $b_1, \ldots, b_m \in \mathbb{R}$ and a positive integer m. Then $x^* \in \mathcal{P}$ is an extreme point of $\mathcal{P}$ if and only if the set

$$\{a_j \mid \langle a_j, x^* \rangle = b_j, j \in \{1, \dots, m\}\}$$

has n linear independent elements.

2.1.3 The cone of positive semidefinite matrices

In this thesis, we will mainly consider the real symmetric matrices space. Let the space of $n \times n$ real symmetric matrices be defined as

$$\mathbb{S}^n := \{X \in \mathbb{R}^{n \times n} \mid X = X^T\},$$

where X^T is the transpose of a matrix X. The inner product over $\mathbb{S}^n$ is the trace inner product: for two matrices $X, Y \in \mathbb{R}^{n \times n}$

$$\langle X, Y \rangle := \mathrm{Tr}(X^T Y) = \sum_{i=1}^{n} \sum_{j=1}^{n} X_{i,j} Y_{i,j},$$

where $\mathrm{Tr}(X) = \sum_{i=1}^{n} X_{i,i}$ is the trace of a matrix $X \in \mathbb{R}^{n \times n}$. Here are some properties of the trace inner product. For matrices $X, Y \in \mathbb{R}^{n \times n}$, we know that $\mathrm{Tr}(XY) = \mathrm{Tr}(YX)$ and $\mathrm{Tr}(X) = \mathrm{Tr}(X^T)$. Let I be the identity matrix and

$$\mathcal{O}^n := \{P \in \mathbb{R}^{n \times n} \mid P^T P = P P^T = I\}$$

be the set of orthogonal matrices. It is easy to verify that $\langle X, Y \rangle = \langle PXP^T, PYP^T \rangle$ holds for matrices $X, Y \in \mathbb{S}^n$ and an orthogonal matrix $P \in \mathcal{O}^n$.

The Frobenius norm of a matrix $X \in \mathbb{R}^{n \times n}$ is defined as:

$$\|X\|_F := \sqrt{\mathrm{Tr}(X^T X)} = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} X_{i,j}^2}.$$

Remark 2.1.5. $\mathbb{S}^n$ can be seen as a $\frac{n(n+1)}{2}$-dimensional Euclidean space, which is a finite dimensional real vector space with an inner product. One can identify the Euclidean space $\mathbb{S}^n$ with $\mathbb{R}^{\frac{n(n+1)}{2}}$ by using the isometry $T : \mathbb{S}^n \to \mathbb{R}^{\frac{n(n+1)}{2}}$ defined by:

$$T(X) = (X_{1,1}, \sqrt{2}X_{1,2}, \dots, \sqrt{2}X_{1,n}, X_{2,2}, \sqrt{2}X_{2,3}, \dots, \sqrt{2}X_{2,n}, \dots, X_{n,n})^T.$$

A matrix $X \in \mathbb{S}^n$ is called positive semidefinite if

$$d^T X d \geq 0 \text{ for every } d \in \mathbb{R}^n.$$

There are some other characterizations of positive semidefinite matrices:

Lemma 2.1.6. (*see, e.g. Theorem 1.10 [13]*) Let $X \in \mathbb{S}^n$. Then the following statements are equivalent:

- X is positive semidefinite.
- All the eigenvalues of X are nonnegative, i.e. the spectral decomposition of X can be written as $X = \sum_{i=1}^{n} \lambda_i p_i p_i^T$ with all $\lambda_i \geq 0$.
- All principal minors of X are nonnegative.

It is useful to know that

Lemma 2.1.7. (*see, e.g. Lemma 1.77 [79]*) Let $X \in \mathbb{S}^n$ and let $P \in \mathcal{O}^n$ be an orthogonal matrix. Then,

$$X \in \mathcal{S}_+^n \text{ if and only if } PXP^T \in \mathcal{S}_+^n.$$

The set of positive semidefinite matrices is denoted as

$$\mathcal{S}_+^n := \{X \in \mathbb{S}^n \mid d^T X d \geq 0 \text{ for any } d \in \mathbb{R}^n\}.$$

$\mathcal{S}_+^n$ is a self-dual proper cone, called the semidefinite cone. It follows from Lemma 2.1.6 that the semidefinite cone can also be expressed as the conical hull of all rank-1 matrices:

$$\mathcal{S}_+^n = \text{cone}(\{xx^T \mid x \in \mathbb{R}^n\}).$$

Example 2.1.8. To give an illustrative explanation of the semidefinite cone, here we consider the specific case:

$$\mathcal{S}_+^2 = \left\{ \begin{pmatrix} a & c \\ c & b \end{pmatrix} \mid a, b, c \in \mathbb{R}, a, b \geq 0,\ ab - c^2 \geq 0 \right\}$$

and draw a figure in $\mathbb{R}^3$ with coordinate a, b and c.

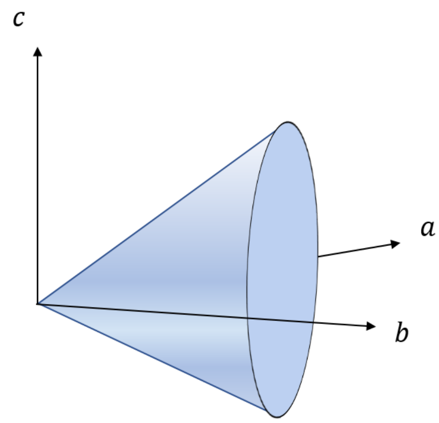


Figure 2.1: The set of $\mathcal{S}_+^2$.

We will illustrate some approximations of the semidefinite cone with Figure 2.1 in Chapter 3.

The semidefinite cone can be used to construct other proper cones. For example, the Doubly NonNegative (DNN) cone is defined as the intersection of $\mathcal{S}_+^n$ and the cone of nonnegative symmetric matrices $\mathcal{N}^n := \{X \in \mathbb{S}^n \mid \forall 1 \le i \le j \le n, X_{i,j} \ge 0\}$:

$$\mathcal{S}_+^n \cap \mathcal{N}^n := \{X \in \mathbb{S}^n \mid X \in \mathcal{S}_+^n, X \in \mathcal{N}^n\},$$

and the Minkowski sum of $\mathcal{S}_+^n$ and $\mathcal{N}^n$ is defined as

$$\mathcal{S}_+^n + \mathcal{N}^n := \{X + Y \mid X \in \mathcal{S}_+^n, Y \in \mathcal{N}^n\}.$$

It is known that $\mathcal{S}_+^n \cap \mathcal{N}^n$ and $\mathcal{S}_+^n + \mathcal{N}^n$ are dual cones of each other (see, e.g., Theorem 1.35 [13] and Proposition 4.1 [121]).

Recently, the copositive cone and its dual cone have attracted much attention in conic optimization. The copositive cone is defined as

$$\mathcal{C}_n := \{X \in \mathbb{S}^n \mid d^T X d \ge 0 \text{ for any } d \in \mathbb{R}_+^n\}.$$

Its dual cone, called the completely positive cone, is given by

$$\mathcal{C}_n^* := \text{cone}(\{xx^T \mid x \in \mathbb{R}_+^n\}).$$

From the definition of each cone, we can see the validity of the following inclusions:

$$\mathcal{C}_n^* \subseteq \mathcal{S}_+^n \cap \mathcal{N}^n \subseteq \mathcal{S}_+^n \subseteq \mathcal{S}_+^n + \mathcal{N}^n \subseteq \mathcal{C}_n.$$

It is known that $\mathcal{N}^n$, $\mathcal{S}_+^n$, $\mathcal{S}_+^n \cap \mathcal{N}^n$ and $\mathcal{C}_n$ are proper cones (see Section 1.6 [13]). Let $\mathcal{K}$ be a proper cone, we know that $\mathcal{K}^*$ is non-empty and pointed (see Proposition 1.18 [13]), closed and convex (Theorem 1.35 [13]), thus proper. Then $\mathcal{S}_+^n + \mathcal{N}^n$ and $\mathcal{C}_n^*$ are also proper cones. Proper cones are essential to construct conic optimization problems, which will be introduced in Section 2.2.

2.2 Conic optimization problems

In recent years, conic optimization has become very popular because it contains many practical classes of problems, such as linear optimization problems, which are computationally efficient and widely used, and semidefinite and copositive optimization problems, which are known as valuable tools for solving combinatorial and nonconvex optimization problems. In this section, we will introduce the general conic optimization problem and its duality theorem.

Let $\mathbb{E}$ be an Euclidean space with an inner product $\langle \cdot, \cdot \rangle$. This inner product defines a norm on $\mathbb{E}$ by $\|x\| = \sqrt{\langle x, x \rangle}$. Then the standard conic optimization problem can be described as the following

$$\begin{aligned} \min\ & \langle c, x \rangle \\ \text{s.t.}\ & \langle a_j, x \rangle = b_j, j = 1, 2, \ldots, m, \\ & x \in \mathcal{K}, \end{aligned} \tag{2.1}$$

where $c, a_j \in \mathbb{E}$, $b_j \in \mathbb{R}$ $(j = 1, \ldots, m)$ and $\mathcal{K} \subseteq \mathbb{E}$ is a proper cone. A point $x \in \mathbb{E}$ is called a feasible solution (respectively, strictly feasible solution) of (2.1) if X satisfies the linear constraints in (2.1) and $x \in \mathcal{K}$ (respectively, $x \in \text{int}(\mathcal{K})$). Here, $\text{int}(\mathcal{K})$ represents the interior of $\mathcal{K}$, i.e., the set of points $y \in \mathcal{K}$ where there exists a positive radius $\delta > 0$ so that the ball centered at y satisfies $\{z \in \mathbb{E} \mid \|y - z\| \leq \delta\} \subseteq \mathcal{K}$.

The dual problem of (2.1) is given by

$$\begin{aligned} \max\ & b^T y \\ \text{s.t.}\ & c - \sum_{j=1}^m y_j a_j = s, \\ & s \in \mathcal{K}^*, \end{aligned} \tag{2.2}$$

where $\mathcal{K}^*$ is the dual cone of $\mathcal{K}$. We say that (y, s) is a feasible solution of (2.2) if $c - \sum_{j=1}^m y_j a_j = s$ and $s \in \mathcal{K}^*$. It is a strict feasible solution if additionally $s \in \mathrm{int}(\mathcal{K}^*)$.

Conic optimization problems contain many useful classes of problems. When the Euclidean space is $\mathbb{R}^n$ with inner product $\langle x, y \rangle = x^T y$, for example, an LP is obtained with $\mathcal{K} = \mathbb{R}^n_+$. If one lets $\mathcal{K}$ be the second-order cone:

$$\mathcal{K} = \{x \in \mathbb{R}^n \mid \sum_{i=1}^{n-1} x_i^2 \leq x_n^2, x_n \geq 0\},$$

then one has an SOCP.

When the Euclidean space is $\mathbb{S}^n$ with the trace inner product, by setting $\mathcal{K} = \mathcal{S}^n_+$, one has an SDP. Moreover, a doubly nonnegative (DNN) optimization problem is given by setting $\mathcal{K} = \mathcal{S}^n_+ \cap \mathcal{N}^n$, and a copositive optimization problem is obtained by letting $\mathcal{K} = \mathcal{C}_n$.

Copositive optimization problems have been shown capable of providing tight lower bounds for combinatorial and quadratic optimization problems, as described in the survey paper by Dür [41] and the recent work of Arima et al. [7, 8, 68], etc. It has been shown that a copositive relaxation sometimes gives a highly accurate approximate solution for some combinatorial problems under certain conditions [9, 27]. However, the copositive program and its dual problem are both NP-hard (see, e.g., [39, 88]). A typical approach in practice is to relax the copositive cone constraint in (2.1) using DNN cone constraint and solve the resulting problem with state-of-the-art SDP solvers.

The strong duality theorem of conic optimization problems is given as follows.

Theorem 2.2.1. (*see, e.g., Theorem 2.29 [22],Theorem 3.2.6 in [97]*) Consider a pair of primal-dual conic optimization problems (2.1) and (2.2), where both the primal and dual problems are strictly feasible. Then both problems have non-empty compact sets of optimal solutions, and there is no duality gap (i.e., the primal and dual objective values are equal).

Remark 2.2.2. It is well-known that for LPs, i.e., by setting $\mathcal{K} = \mathbb{R}^n_+$ in (2.1) and (2.2), we have a more attractive duality theorem (see, e.g., Theorem 2.1 [119]): If both the primal and dual problems are feasible, then both problems have optimal solutions, and the objective values are equal.

Chapter 3

Approximations of the semidefinite cone

A set $\mathcal{S}$ is called an outer approximation of $\mathcal{S}^n_+$ if $\mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathbb{S}^n$. Similarly, a set $\mathcal{S}$ which satisfies $\mathcal{S} \subseteq \mathcal{S}^n_+$ is called an inner approximation of $\mathcal{S}^n_+$. Several sets have been used as inner and outer approximations of the semidefinite cone. In this chapter, we introduce some common approximations of the semidefinite cone, i.e., $\mathcal{FW}_n(k)$, $\mathcal{S}^{n,k}$, $\mathcal{DD}_n$, $\mathcal{SDD}_n$ and $\text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-)$, and their properties. Then we propose a new polyhedral approximation of the semidefinite cone using a set of parameters, i.e., $\mathcal{SDB}_n(\mathcal{H})$ where $\mathcal{H} \subseteq \mathbb{R}$. We prove several essential properties of our new polyhedral approximation and show that $\text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-) = \mathcal{DD}_n$ and $\mathcal{SDB}_n(\mathbb{R}) = \mathcal{SDD}_n$. With these results, Corollary 3.2.7 gives the inclusive relation among all approximations mentioned in this thesis.

The organization of this chapter is as follows. In Section 3.1, we list five different approximations, including those based on factor width by Boman et al. [23] and Blekherman et al. [20], diagonal dominance by Ahmadi et al. [1], and SD bases by Tanaka and Yoshise [106]. In Section 3.2, we propose an expansion of SD bases and construct new polyhedral approximations using expanded SD bases. We also discuss how to increase the "volume" of these new polyhedral approximations. Finally, we conclude our work in Section 3.3. The contents in this chapter are based on the published study [114].

3.1 Some approximations of the semidefinite cone

In this section, we first introduce the concept of factor width. Then the inner and outer approximations of $\mathcal{S}^n_+$ based on the factor width, specifically $\mathcal{FW}_n(k)$ and $\mathcal{S}^{n,k}$, and their properties are discussed. Then we consider inner and outer approximations of $\mathcal{S}^n_+$ using diagonal dominance, specifically $\mathcal{DD}_n$, $\mathcal{SDD}_n$ and their dual cones. The characterizations and the inclusive relation of those approximations are also discussed. Finally, we introduce the SD bases $\mathcal{B}^n_+$ and $\mathcal{B}^n_-$ and shows that $\text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-) = \mathcal{DD}_n$.

3.1.1 Approximations using factor width

Several approximations of the semidefinite cone are constructed using a concept called factor width, including the set of matrices with a factor width of at most k: $\mathcal{FW}_n(k)$ by Boman et al. [23], its dual cone $\mathcal{S}^{n,k}$ by Blekherman et al. [20], and an extension of $\mathcal{FW}_n(k)$ using matrix block partition by Zheng et al [124]. In this section, we introduce the concept of factor width and two approximations using it: $\mathcal{FW}_n(k)$ and $\mathcal{S}^{n,k}$.

In [23], Boman et al. defined a concept called factor width.

Definition 3.1.1. (*Definition 1 in [23]*) The factor width of a real symmetric matrix $A \in \mathbb{S}^n$ is the smallest integer k such that there exists a real matrix $V \in \mathbb{R}^{n\times m}$ where $A = VV^T$ and each column of V contains at most k nonzero elements.

Here is an example of a matrix with a factor width of at most 2 in $\mathbb{S}^3$:

Example 3.1.2. If we let

$$A = \begin{pmatrix} 2 & -1 & -2 \\ -1 & 5 & 2 \\ -2 & 2 & 6 \end{pmatrix},\ V = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ -2 & 0 & 1 & 1 \end{pmatrix},$$

then we can find that $A = VV^T$, and V has at most two nonzero elements in each column. This implies that A has a factor width of at most two.

Note that the factor width is only defined for semidefinite matrices, because for every matrix A in Definition 3.1.1, the decomposition $A = VV^T$ implies that $A \in \mathcal{S}^n_+$. Then for every $k \in \{1, 2, \ldots, n\}$, the set of matrices with a factor width of at most k gives an inner approximation of $\mathbb{S}^n_+$.

Boman et al. [23] also defined the set of matrices with a factor width of at most k.

Definition 3.1.3. *([23])* Let k and n be positive integers where $1 \le k \le n$. The set of matrices with a factor width of at most k is defined as

$$\mathcal{FW}_n(k) := \{X \in \mathbb{S}^n \mid \text{X has a factor width of at most } k\}.$$

It is easy to verify that $\mathcal{FW}_n(k)$ is a pointed convex cone for any $k \in \{1, 2, \ldots, n\}$. One can also verify from Definition 3.1.3 that $\mathcal{FW}_n(k_1) \subseteq \mathcal{FW}_n(k_2)$ when $1 \le k_1 \le k_2 \le n$ and $\mathcal{FW}_n(n) = \{X \in \mathbb{S}^n \mid \exists V \in \mathbb{R}^{n\times m}, X = VV^T\} = \mathcal{S}^n_+$. In conclusion, for $n \ge 2$ we have

$$\mathcal{FW}_n(1) \subseteq \mathcal{FW}_n(2) \subseteq \ldots \subseteq \mathcal{FW}_n(n) = \mathcal{S}^n_+.$$

We give an illustration of $FW_n(2)$, $FW_n(3)$ and the semidefinite cone when $n = 10$ to show the inclusive relation among them explicitly in the following example.

Example 3.1.4. Let I be the identity matrix in $\mathbb{S}^{10}$. We randomly generate two matrices $A, B \in \mathbb{S}^{10}$, whose entries are taken independently from the uniform distribution on the interval $[-0.5, 0.5]$. For given scalars $\alpha, \beta \in \mathbb{R}$, we check whether the matrix $I + \alpha A + \beta B$ is in $\mathcal{FW}_{10}(2)$, $\mathcal{FW}_{10}(3)$ and $\mathcal{S}^{10}_+$. Let $\mathcal{G}_{A,B}(\mathcal{S}) := \{(\alpha, \beta) \in \mathbb{R}^2 \mid I + \alpha A + \beta B \in \mathcal{S}\}$. Figure 3.1 shows the region of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{FW}_{10}(2), \mathcal{FW}_{10}(3), \mathcal{S}^{10}_+\}$.

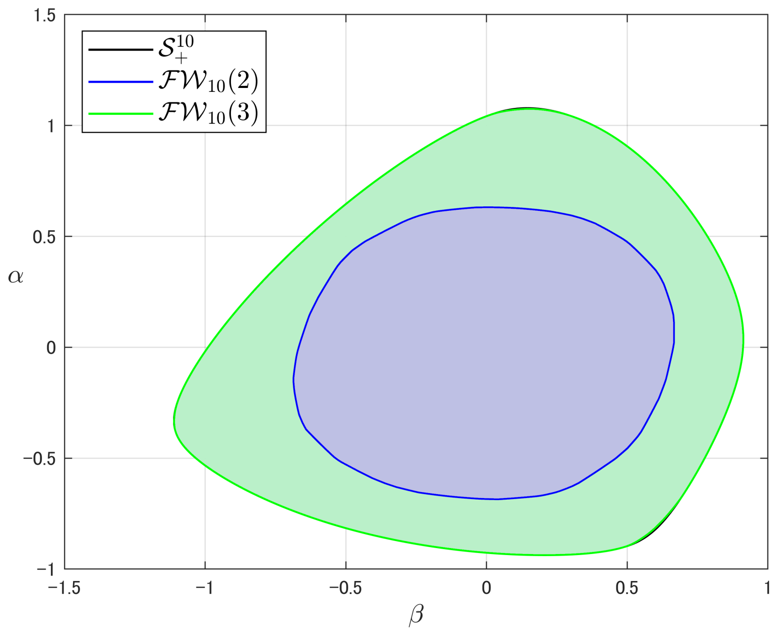


Figure 3.1: Figure of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{FW}_{10}(2), \mathcal{FW}_{10}(3), \mathcal{S}^{10}_+\}$.

We next give an explicit characterization of $\mathcal{FW}_n(k)$ and a simple proof for completeness.

Lemma 3.1.5. (*Characterization of* $\mathcal{FW}_n(k)$) Let k and n be positive integers where $1 \leq k \leq n$. Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere, and let $E_{\mathcal{I}} = (e_{i_1}, e_{i_2}, \dots, e_{i_k}) \in \mathbb{R}^{n \times k}$ for any index set $\mathcal{I} := \{i_1, \dots, i_k\} \subseteq \{1, \dots, n\}$ where $i_1 < \cdots < i_k$. Then we can explicitly characterize $\mathcal{FW}_n(k)$ as follows:

$$\mathcal{FW}_n(k) = \left\{ \sum_{\substack{\mathcal{I} := \{i_1, \dots, i_k\} \subseteq \{1, \dots, n\} \\ i_1 < \cdots < i_k}} E_{\mathcal{I}} X_{\mathcal{I}} E_{\mathcal{I}}^T \mid X_{\mathcal{I}} \in \mathcal{S}^k_+ \right\}.$$

Proof. For any matrix $X = \sum_{\substack{\mathcal{I} \subseteq \{1, \dots, n\} \\ i_1 < \cdots < i_k}} E_{\mathcal{I}} X_{\mathcal{I}} E_{\mathcal{I}}^T$ where $X_{\mathcal{I}} \in \mathcal{S}^k_+$, we know that there exists

$V_{\mathcal{I}} \in \mathbb{R}^{k\times m}$ for some m such that $X_{\mathcal{I}} = V_{\mathcal{I}} V_{\mathcal{I}}^T$. Then $X = \sum_{\substack{\mathcal{I}\subseteq\{1,\dots,n\}\\ i_1<\dots<i_k}} (E_{\mathcal{I}} V_{\mathcal{I}})(E_{\mathcal{I}} V_{\mathcal{I}})^T$. Since $E_{\mathcal{I}} V_{\mathcal{I}} \in \mathbb{R}^{n\times m}$ and each column contains at most k nonzero elements, we know that $X \in \mathcal{FW}_n(k)$.

For any matrix $X \in \mathcal{FW}_n(k)$, by Definition 3.1.3, we know that X has a decomposition $X = \sum_{i=1}^m v_i v_i^T$ where v_i has at most k nonzero element for all $i = 1, \dots, m$. Let $\mathcal{J}_i := \{j_1, \dots, j_k\}$ be the set of k indexes including the indexes of nonzero elements of v_i where $j_1 < \dots < j_k$. Then for every $i = 1, \dots, m$, we have

$$v_i v_i^T = E_{\mathcal{J}} \begin{pmatrix} v_{j_1}^2 & \cdots & v_{j_1} v_{j_k} \\ \vdots & \ddots & \vdots \\ v_{j_k} v_{j_1} & \cdots & v_{j_k}^2 \end{pmatrix} E_{\mathcal{J}}^T.$$

The $k \times k$ matrix on the right-hand side between $E_{\mathcal{J}}$ and $E_{\mathcal{J}}^T$ is positive semidefinite, which implies that

$$X = \sum_{i=1}^m v_i v_i^T \in \left\{ \sum_{\substack{\mathcal{I}:=\{i_1,\dots,i_k\}\subseteq\{1,\dots,n\}\\ i_1<\dots<i_k}} E_{\mathcal{I}} X_{\mathcal{I}} E_{\mathcal{I}}^T \mid X_{\mathcal{I}} \in \mathcal{S}_+^k \right\}.$$

□

Here is an example of the above characterization of the matrix in Example 3.1.2:

Example 3.1.6. Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere, and define $E_{\{i,j\}} := (e_i, e_j)$. Let

$$A = \begin{pmatrix} 2 & -1 & -2 \\ -1 & 5 & 2 \\ -2 & 2 & 6 \end{pmatrix}.$$

Then A can be characterized as follows:

$$A = E_{\{1,2\}} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} E_{\{1,2\}}^T + E_{\{1,3\}} \begin{pmatrix} 1 & -2 \\ -2 & 4 \end{pmatrix} E_{\{1,3\}}^T + E_{\{2,3\}} \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix} E_{\{2,3\}}^T,$$

where all the 2×2 matrices above are positive semidefinite. This implies that $A \in \mathcal{FW}_3(2)$.

Another approximation of the semidefinite cone based on factor width is the *k-PSD closure*, whose properties are discussed in [20]. The definition of the *k-PSD closure* is given as follows.

Definition 3.1.7. (Definition 1 in [20]) Given positive integers n and k where $1 \leq k \leq n$, the *k-PSD closure*, denoted as $\mathcal{S}^{n,k}$, is defined as

$$\mathcal{S}^{n,k} := \{X \in \mathbb{S}^n \mid \text{ All } k \times k \text{ principal submatrices of } X \text{ are positive semidefinite}\}.$$

Here is an example of the matrix in $\mathcal{S}^{3,2}$.

Example 3.1.8. If we let

$$A = \begin{pmatrix} 4 & -2 & 6 \\ -2 & 1 & 3 \\ 6 & 3 & 9 \end{pmatrix},$$

then we can see that every 2×2 principal submatrix of A is positive semidefinite, which implies that $A \in \mathcal{S}^{3,2}$. One can verify that the determinant of A is negative: $|A| < 0$, showing that $A \notin \mathcal{S}^3_+$.

$\mathcal{S}^{n,k}$ is a pointed convex cone for any $1 \leq k \leq n$. and it is obvious from Definition 3.1.7 that $\mathcal{S}^n_+ = \mathcal{S}^{n,n} \subseteq \mathcal{S}^{n,k_2} \subseteq \mathcal{S}^{n,k_1}$ when $1 \leq k_1 \leq k_2 \leq n$. Then for every $k \in \{1, 2, \ldots, n\}$, the *k-PSD closure* gives an outer approximation of the semidefinite cone.

Similar to Lemma 3.1.5, the following characterization of $\mathcal{S}^{n,k}$ using operator $E_{\mathcal{I}}$ is straightforward.

Lemma 3.1.9. (*Characterization of* $\mathcal{S}^{n,k}$) Let k and n be positive integers where $1 \leq k \leq n$. Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere, and let $E_{\mathcal{I}} := (e_{i_1}, e_{i_2}, \ldots, e_{i_k}) \in \mathbb{R}^{n \times k}$ for any index set $\mathcal{I} := \{i_1, \ldots, i_k\} \subseteq \{1, \ldots, n\}$ where $i_1 < \cdots < i_k$. Then

$$\mathcal{S}^{n,k} = \left\{ X \in \mathbb{S}^n \mid \forall \mathcal{I} := \{i_1, \ldots, i_k\} \subseteq \{1, \ldots, n\}, i_1 < \cdots < i_k, \quad E_{\mathcal{I}}^T X E_{\mathcal{I}} \in \mathcal{S}^k_+ \right\}.$$

It is also easy to see from Lemma 3.1.5 and 3.1.9 that $\mathcal{FW}_n(k)$ and $\mathcal{S}^{n,k}$ are dual cones of each other:

Lemma 3.1.10. For any $1 \leq k \leq n$,

$$(\mathcal{FW}_n(k))^* = \mathcal{S}^{n,k}, \ (\mathcal{S}^{n,k})^* = \mathcal{FW}_n(k).$$

By Lemma 3.1.5 and 3.1.9, checking whether a matrix is in $\mathcal{FW}_n(k)$ or $\mathcal{S}^{n,k}$ requires to solve a semidefinite optimization problem with $C_n^k := \frac{n!}{k!(n-k)!}$ semidefinite constraints of size k, which seems to be inefficient for $k \geq 3$. Thus in practice, $\mathcal{FW}_n(k)$ and $\mathcal{S}^{n,k}$ are used to solve SDPs by setting $k \leq 2$. We refer to Zheng et al. [124] for an extension of $\mathcal{FW}_n(k)$ using the matrix block partition, which aims to alleviate the deficiency mentioned above.

3.1.2 Approximations using diagonal dominance

In [1] and [2], the authors approximated the cone $\mathcal{S}^n_+$ with the set of diagonally dominant matrices and the set of scaled diagonally dominant matrices. In this section, we introduce these two sets and their relation to other common sets.

The set of diagonally dominant matrices $\mathcal{DD}_n$ are defined as follows:

Definition 3.1.11. (*Definition 6.1.9 in [59]*)

$$\mathcal{DD}_n := \{A \in \mathbb{S}^n \mid \ A_{i,i} \geq \sum_{j \neq i} |A_{i,j}| \quad (i = 1, 2, \ldots, n)\}.$$

Note that the above definition uses weak inequalities, and a matrix satisfying weak inequalities in the above definition is sometimes called a weak diagonally dominant matrix. Similarly, a matrix satisfying strict inequalities in Definition 3.1.11 is sometimes called a strict diagonally dominant matrix. In this paper, we only consider weak inequalities and call matrices in $\mathcal{DD}_n$ diagonally dominant matrices.

Ahmadi et al. [1] defined $\bar{\mathcal{U}}_{n,k}$ as the set of vectors in $\mathbb{R}^n$ with at most k nonzeros, each equal to 1 or -1. They also defined a set of matrices $\mathcal{U}_{n,k} := \{uu^T \mid u \in \bar{\mathcal{U}}_{n,k}\}$. Barker and Carlson [10] proved the following theorem.

Theorem 3.1.12. *(Barker and Carlson [10])* $\mathcal{DD}_n = \text{cone}(\mathcal{U}_{n,2})$.

It is easy to see that $\mathcal{DD}_n$ is a convex cone, and Theorem 3.1.12 implies that $\mathcal{DD}_n$ has n^2 extreme rays; thus, it is a finitely generated cone. By Theorem 2.1.3, we know that $\mathcal{DD}_n$ is a polyhedral cone.

Here is an example of a matrix in $\mathcal{DD}_n$ and its characterization.

Example 3.1.13. Let

$$A = \begin{pmatrix} 4 & -2 & 1 \\ -2 & 3 & 1 \\ 1 & 1 & 2 \end{pmatrix},$$

and let

$$u_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \ u_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, u_3 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}.$$

One can see that

$$A = 2u_1u_1^T + u_2u_2^T + u_3u_3^T \in \text{cone}(\mathcal{U}_{3,2}) = \mathcal{DD}_3.$$

Using the characterization in Theorem 3.1.12, we can give a characterization of the dual cone of $\mathcal{DD}_n$.

Corollary 3.1.14. (*Characterization of* $\mathcal{DD}_n^*$)

$$\mathcal{DD}_n^* = \{X \in \mathbb{S}^n \mid \langle X, Y\rangle \geq 0, \forall Y \in \mathcal{U}_{n,2}\}.$$

As an extension of the set of diagonally dominant matrix, the set of scaled diagonally dominant matrices $\mathcal{SDD}_n$ are defined as follows:

Definition 3.1.15. (*Definition 3.3 in [1]*)

$$\mathcal{SDD}_n := \{A \in \mathbb{S}^n \mid DAD \in \mathcal{DD}_n \textit{ for some positive diagonal matrix } D\}.$$

One can easily see that $\mathcal{SDD}_n$ is a cone in $\mathbb{S}^n$. Here is an example of a matrix in $\mathcal{SDD}_n$.

Example 3.1.16. Let

$$A = \begin{pmatrix} 4 & -6 & 1 \\ -6 & 27 & 3 \\ 1 & 3 & 2 \end{pmatrix}.$$

One can verify that

$$A = \begin{pmatrix} 1 & & \\ & 3 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 4 & -2 & 1 \\ -2 & 3 & 1 \\ 1 & 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & & \\ & 3 & \\ & & 1 \end{pmatrix}.$$

By Example 3.1.13, we know that the matrix in the middle of the right-hand side is diagonally dominant. Thus we have $A \in \mathcal{SDD}_n$.

The following lemma is a well-known result, which is a consequence of the Gershgorin circle theorem ([47], see also Theorem 6.1.1 in [59]).

Lemma 3.1.17. *(Relation among $\mathcal{DD}_n, \mathcal{SDD}_n$, and $\mathcal{S}^n_+$, see Ahmadi et al. [1])*

$$\mathcal{DD}_n \subseteq \mathcal{SDD}_n \subseteq \mathcal{S}^n_+.$$

Example 3.1.18. Let I be the identity matrix in $\mathbb{S}^{10}$. We use the same matrices $A, B \in \mathbb{S}^{10}$ generated in Example 3.1.4. For given scalars $\alpha, \beta \in \mathbb{R}$, we check whether the matrix $I + \alpha A + \beta B$ is in $\mathcal{DD}_{10}$, $\mathcal{SDD}_{10}$ and $\mathcal{S}^{10}_+$. Let $\mathcal{G}_{A,B}(\mathcal{S}) := \{(\alpha, \beta) \in \mathbb{R}^2 \mid I + \alpha A + \beta B \in \mathcal{S}\}$. Figure 3.2 shows the region of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{DD}_{10}, \mathcal{SDD}_{10}, \mathcal{S}^{10}_+\}$.

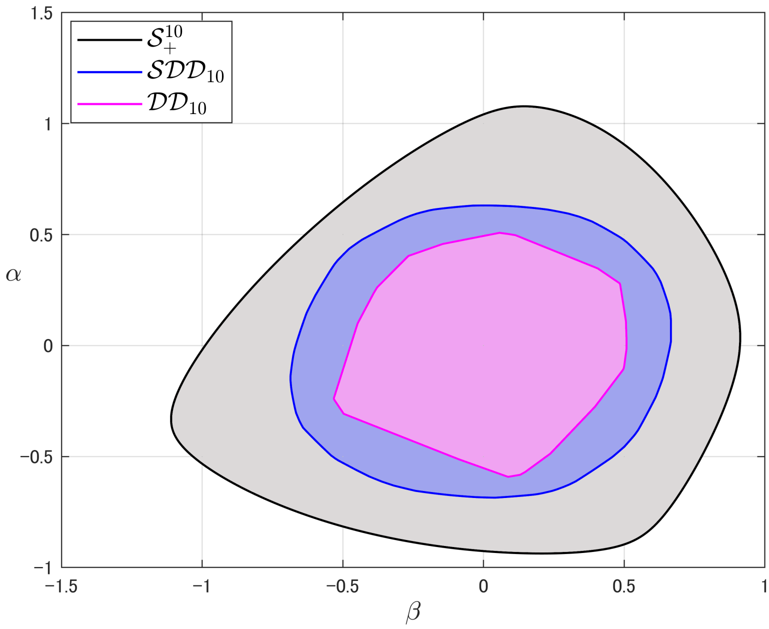


Figure 3.2: Figure of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{DD}_{10}, \mathcal{SDD}_{10}, \mathcal{S}^{10}_+\}$.

Note that Ahmadi et al. [1, 2] showed that the problem of optimizing a linear function over $\mathcal{DD}_n$ can be solved as LPs. They also proved that the problem of optimizing a linear function over $\mathcal{SDD}_n$ can be solved as SOCPs. They designed a column generation method using $\mathcal{DD}_n$ and $\mathcal{SDD}_n$ to obtain a series of inner approximations of $\mathcal{S}^+_n$. As its extension, Gouveia et al. [51] used $\mathcal{SDD}_n$ to inner approximate the completely positive cone.

In [23] and in [2], a relation between $\mathcal{SDD}_n$ and $\mathcal{FW}_n(2)$ is given:

Lemma 3.1.19. *(See [23] and Theorem 8 in [2])* For $n \geq 2$,

$$\mathcal{FW}_n(2) = \mathcal{SDD}_n.$$

Note that Definition 3.1.3 implies that the set $\mathcal{FW}_n(k)$ is convex for any $k \in \{1, 2, \ldots, n\}$, and we know that the set $\mathcal{SDD}_n$ is a convex cone. From Lemma 3.1.19 and Lemma 3.1.10, we know the equivalence between the dual cone of $\mathcal{SDD}_n$ and $\mathcal{S}^{n,2}$:

Corollary 3.1.20. For $n \geq 2$,

$$\mathcal{SDD}_n^* = \mathcal{S}^{n,2}.$$

3.1.3 Approximations using SD basis

Unlike the previous approximations of $\mathcal{S}_+^n$, the one in this section considers the conical hull of a basis on $\mathbb{S}^n$. Note that the semidefinite cone can be expressed as the conical hull of all rank-1 matrices:

$$\mathcal{S}_+^n = \text{cone}(\{xx^T \mid x \in \mathbb{R}^n\}).$$

The approximation of $\mathcal{S}_+^n$ by using SD bases considers the convex cone generated by a finite number of rank-1 semidefinite matrices. That is, given a subset of rank-1 matrices, $\mathcal{B} \subseteq \{xx^T \mid x \in \mathbb{R}^n\}$, an inner polyhedral approximation of $\mathcal{S}_+^n$ can be obtained from cone($\mathcal{B}$):

$$\text{cone}(\mathcal{B}) \subseteq \text{cone}(\{xx^T \mid x \in \mathbb{R}^n\}) = \mathcal{S}_+^n.$$

To obtain the original set $\mathcal{S}_+^n$, we would have to add an infinite number of matrices to the set $\mathcal{B}$, which is not efficient from a computational viewpoint. Instead, to generate a polyhedral approximation with reasonable accuracy by using limited elements, Tanaka and Yoshise defined semidefinite (SD) bases [106].

Before introducing SD bases, we first need a fundamental result by Dickinson [40].

Lemma 3.1.21. *(Lemma 6.2 in [40])* If $\{p_1, ..., p_n\}$ is a set of n linearly independent vectors, then $\{(p_i + p_j)(p_i + p_j)^T \mid 1 \leq i \leq j \leq n\}$ is a set of $\frac{n(n+1)}{2}$ linearly independent symmetric matrices.

Then we introduce the semidefinite (SD) bases defined by Tanaka and Yoshise [106].

Definition 3.1.22. *(Definitions 1 and 2 in [106])* Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere. Then

$$\mathcal{B}_+^n := \{(e_i + e_j)(e_i + e_j)^T \mid 1 \leq i \leq j \leq n\}$$

is called an SD basis of Type I, and

$$\mathcal{B}_-^n := \{(e_i + e_i)(e_i + e_i)^T \mid 1 \leq i \leq n\} \cup \{(e_i - e_j)(e_i - e_j)^T \mid 1 \leq i < j \leq n\}$$

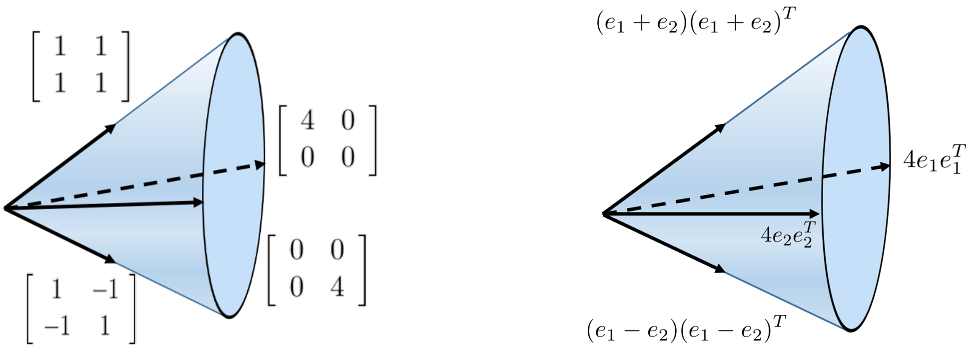
is called an SD basis of Type II. Matrices in SD bases Type I and II are defined as

$$B_{i,j}^+ := (e_i + e_j)(e_i + e_j)^T, \; B_{i,j}^- := (e_i - e_j)(e_i - e_j)^T.$$

Example 3.1.23. As an example in $\mathbb{S}^2$, let $e_1 = (1,0)^T$ and $e_2 = (0,1)^T$. Then, we can generate the following SD bases of Types I and II, respectively:

$$\mathcal{B}_+^2 = \left\{ \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix} \right\},$$
$$\mathcal{B}_-^2 = \left\{ \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix} \right\}.$$

Figure 3.3 shows how the matrices of these SD bases lie on the boundary of $\mathcal{S}_+^n$.



[a] An example of matrices in $\mathcal{B}_+^2 \cup \mathcal{B}_-^2$ [b] Characterization of matrices in $\mathcal{B}_+^2 \cup \mathcal{B}_-^2$.

Figure 3.3: An example of SD bases in $\mathbb{S}^2$

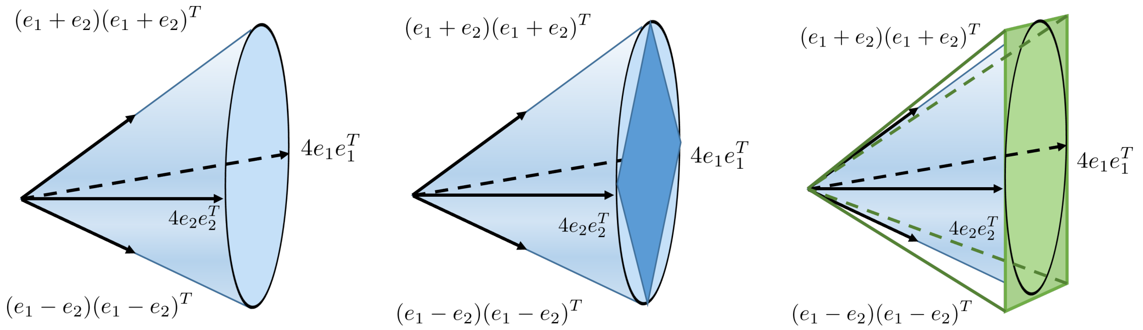
As shown in [106], $\mathcal{B}_+^n$ and $\mathcal{B}_-^n$ are subsets of $\mathcal{S}_+^n$ and bases of $\mathbb{S}^n$. The conical hull of $\mathcal{B}_+^n \cup \mathcal{B}_-^n$ and its dual cone give an inner and an outer polyhedral approximation of $\mathcal{S}_+^n$, as follows.

Definition 3.1.24. The inner and outer approximations of $\mathcal{S}_+^n$ by using SD bases are defined as

$$\begin{aligned}\mathcal{S}^n_{\text{in}} :=& \text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-),\\ \mathcal{S}^n_{\text{out}} :=& (\mathcal{S}_{\text{in}})^*\\ =& \{X \in \mathbb{S}^n \mid \langle X, Y\rangle \geq 0, \forall Y \in \mathcal{B}^n_+ \cup \mathcal{B}^n_-\}.\end{aligned}$$

By Definition 3.1.22, we know that $\mathcal{B}^n_+, \mathcal{B}^n_- \subseteq \mathcal{S}^n_+$. Since $\mathcal{S}^n_+$ is a convex cone, we have $\mathcal{S}^n_{\text{in}} \subseteq \text{cone}(\mathcal{S}^n_+) = \mathcal{S}^n_+$. By Lemma 1.7.3 in [79], we know that $\mathcal{S}^n_+$ is self-dual; that is, $\mathcal{S}^n_+ = (\mathcal{S}^n_+)^*$. Accordingly, we can conclude that $\mathcal{S}^n_{\text{in}} \subseteq \mathcal{S}^n_+ \subseteq \mathcal{S}^n_{\text{out}}$.

Example 3.1.25. Let $\mathcal{B}^2_+$ and $\mathcal{B}^2_-$ be SD basis of type I and II as in Example 3.1.23. Figure 3.4 [b] (respectively, [c]) gives an illustration of the intersection between hyperplane $\{X \in \mathbb{S}^n \mid \text{Tr}(X) = 4\}$ and the inner (respectively, outer) approximations $\mathcal{S}^2_{\text{in}}$ (respectively, $\mathcal{S}^2_{\text{out}}$).



[a] SD bases $\mathcal{B}^2_+ \cup \mathcal{B}^2_-$. [b] Inner approximation $\mathcal{S}^2_{\text{in}}$ using $\mathcal{B}^2_+ \cup \mathcal{B}^2_-$. [c] Outer approximation $\mathcal{S}^2_{\text{out}}$ using $\mathcal{B}^2_+ \cup \mathcal{B}^2_-$.

Figure 3.4: An example of polyhedral approximations of $\mathcal{S}^2_+$ using SD bases

In [106], $\mathcal{B}^n_+$ and $\mathcal{B}^n_-$ are defined as $\mathcal{B}^n_+(P)$ and $\mathcal{B}^n_-(P)$ using an orthogonal matrix P. In fact, for any orthogonal matrix P,

$$\begin{aligned}\mathcal{B}^n_+(P) :=& P\mathcal{B}^n_+P^T = \{PB^+_{i,j}P^T \mid B^+_{i,j} \in \mathcal{B}^n_+\},\\ \mathcal{B}^n_-(P) :=& P\mathcal{B}^n_-P^T = \{PB^-_{i,j}P^T \mid B^-_{i,j} \in \mathcal{B}^n_-\}\end{aligned}$$

give generalizations of $\mathcal{B}^n_+$ and $\mathcal{B}^n_-$, which are bases on $\mathbb{S}^n$ as well. Note that $\mathcal{B}^n_+ = \mathcal{B}^n_+(I)$ and $\mathcal{B}^n_- = \mathcal{B}^n_-(I)$ hold, where I is the identity matrix. Here is an example of this generalization.

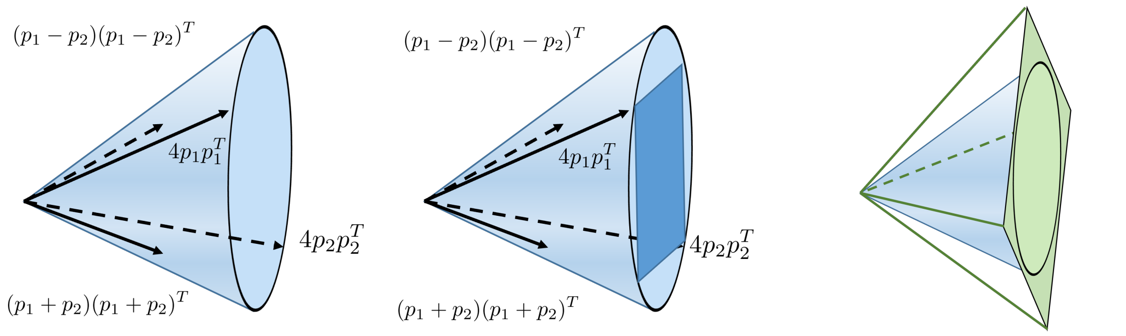
Example 3.1.26. Let $\mathcal{B}^n_+$ and $\mathcal{B}^n_-$ be defined as in Example 3.1.23, and let $P = (p_1, p_2)$ be an orthogonal matrix where

$$p_1 = \begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{pmatrix}, p_2 = \begin{pmatrix} \frac{-2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix}.$$

Then we have

$$\begin{aligned} \mathcal{B}_+^n(P) &= \left\{ \begin{pmatrix} \frac{4}{5} & \frac{8}{5} \\ \frac{8}{5} & \frac{16}{5} \end{pmatrix}, \begin{pmatrix} \frac{1}{5} & \frac{-3}{5} \\ \frac{-3}{5} & \frac{9}{5} \end{pmatrix}, \begin{pmatrix} \frac{16}{5} & \frac{-8}{5} \\ \frac{-8}{5} & \frac{4}{5} \end{pmatrix} \right\}, \\ \mathcal{B}_-^n(P) &= \left\{ \begin{pmatrix} \frac{4}{5} & \frac{8}{5} \\ \frac{8}{5} & \frac{16}{5} \end{pmatrix}, \begin{pmatrix} \frac{9}{5} & \frac{3}{5} \\ \frac{3}{5} & \frac{1}{5} \end{pmatrix}, \begin{pmatrix} \frac{16}{5} & \frac{-8}{5} \\ \frac{-8}{5} & \frac{4}{5} \end{pmatrix} \right\}. \end{aligned}$$

Figure 3.5 [a] shows the matrices in $\mathcal{B}_+^n(P) \cup \mathcal{B}_-^n(P)$ and Figure 3.5 [b] (respectively, [c]) gives an illustration of the intersection between hyperplane $\{X \in \mathbb{S}^n \mid \text{Tr}(X) = 4\}$ and the inner (respectively, outer) approximation using $\mathcal{B}_+^n(P) \cup \mathcal{B}_-^n(P)$ in $\mathbb{S}^2$.



[a] Generalization of SD bases $\mathcal{B}_+^n(P) \cup \mathcal{B}_-^n(P)$.

[b] Inner approximation using $\mathcal{B}_+^n(P) \cup \mathcal{B}_-^n(P)$.

[c] Outer approximation using $\mathcal{B}_+^n(P) \cup \mathcal{B}_-^n(P)$.

Figure 3.5: An example of polyhedral approximations of $\mathcal{S}_+^2$ using the generalization of SD bases

Next, we give a lemma that provides an expression of $\mathcal{S}_+^n$ by using SD bases. The lemma is a direct result of the fact that any $X \in \mathcal{S}_+^n$ has nonnegative eigenvalues and a corresponding orthogonal basis of eigenvectors.

Lemma 3.1.27. Let $\mathcal{O}^n$ be the set of all $n \times n$ orthogonal matrices. Then

$$\mathcal{S}_+^n = \text{cone}\left(\bigcup_{P \in \mathcal{O}^n} \{P^T X P \mid X \in \mathcal{B}_+^n\} \right) = \text{cone}\left(\bigcup_{P \in \mathcal{O}^n} \{P^T X P \mid X \in \mathcal{B}_-^n\} \right).$$

Lemma 3.1.27 gives a way to approximate $\mathcal{S}_+^n$ by changing the matrix $P = (p_1, .., p_n)$

$\in \mathcal{O}^n$ when creating SD bases. However, a dense matrix $P \in \mathcal{O}^n$ may lead to a dense formulation of the approximation using SD basis, which is unattractive from the standpoint of computational efficiency.

In fact, if we consider the following relaxed problem using the generalizations $P\mathcal{B}_+^n P^T$:

$$\begin{aligned} &\min \ \langle C, X\rangle \\ &\text{s.t.}\ \langle A_j, X\rangle = b_j,\ \forall j = 1,\dots,m, \\ &\qquad \langle Y, X\rangle \geq 0, \quad \forall Y \in P\mathcal{B}_+^n P^T, \end{aligned}$$

where $C, A_j \in \mathbb{S}^n$, $b_j \in \mathbb{R}$ $(j = 1,\dots,m)$. One can see that it is equivalent to the following problem

$$\begin{aligned} &\min \ \langle C, X\rangle \\ &\text{s.t.}\ \langle A_j, X\rangle = b_j,\ \forall j = 1,\dots,m, \\ &\qquad \langle PYP^T, X\rangle \geq 0, \quad \forall Y \in \mathcal{B}_+^n, \end{aligned}$$

By setting $\bar{X} := P^T XP$, the problem is furthermore equivalent to

$$\begin{aligned} &\min \ \langle P^T CP, \bar{X}\rangle \\ &\text{s.t.}\ \langle P^T A_j P, \bar{X}\rangle = b_j,\ \forall j = 1,\dots,m, \\ &\qquad \langle Y, \bar{X}\rangle \geq 0, \quad \forall Y \in \mathcal{B}_+^n. \end{aligned} \tag{3.1}$$

Therefore, we consider that the generalizations $P\mathcal{B}_+^n P^T$ and $P\mathcal{B}_+^n P^T$ are not essential throughout this thesis and omit those descriptions from subsequent sections to simplify the presentation.

Next, as a corollary of Theorem 3.1.12, we give the relation between $\mathcal{DD}_n$ and SD bases. A proof is given here for completeness.

Corollary 3.1.28. *(Expression of $\mathcal{DD}_n$ with SD bases)*

$$\text{cone}(\mathcal{B}_+^n \cup \mathcal{B}_-^n) = \mathcal{DD}_n.$$

Proof. Let $I = (e_1,\dots,e_n) \in \mathbb{S}^n$ be the identity matrix. $\forall X \in \mathcal{DD}_n \subseteq \mathbb{S}^n$, we first define a matrix $X^1 \in \mathbb{S}^n$:

$$\begin{aligned} X^1 \ &:= \sum_{1\leq i<j\leq n} |X_{i,j}|(e_i + \text{sgn}(X_{i,j})e_j)(e_i + \text{sgn}(X_{i,j})e_j)^T \\ &\in \ \text{cone}\left(\mathcal{B}_+^n \cup \mathcal{B}_-^n\right) \ \text{(because } \forall i < j, |X_{i,j}| \geq 0), \end{aligned} \tag{3.2}$$

where $\mathrm{sgn}(X_{i,j})$ is the sign function, i.e.,

$$\mathrm{sgn}(X_{i,j}) := \begin{cases} 1 & (X_{i,j} \geq 0), \\ -1 & (\text{otherwise}) \end{cases}$$

From (3.2), it is obvious that $\forall i \neq j, X^1_{i,j} = X_{i,j}$. As for the diagonal entries of X^1, $\forall i = 1, .., n$,

$$\begin{aligned} X^1_{i,i} &= \sum_{i<j} |X_{i,j}| + \sum_{i>j} |X_{j,i}| \text{ (by (3.2))} \\ &= \sum_{i \neq j} |X_{i,j}| \text{ (because } X \in \mathcal{DD}_n \subseteq \mathbb{S}^n). \end{aligned}$$

As $X \in \mathcal{DD}_n$, we know from Definition 3.1.11 that $\forall i = 1, .., n$,

$$X_{i,i} - X^1_{i,i} = X_{i,i} - \sum_{i \neq j} |X_{i,j}| \geq 0.$$

Then, we define another matrix $X^2 \in \mathbb{S}^n$:

$$\begin{aligned} X^2 &:= \sum_{i=1,..,n} \frac{X_{i,i} - \sum_{i \neq j} |X_{i,j}|}{4} (e_i + e_i)(e_i + e_i)^T \\ &\in \mathrm{cone}\left(\mathcal{B}^n_+ \cup \mathcal{B}^n_-\right) \text{ (because } \forall i = 1, .., n, X_{i,i} - \sum_{i \neq j} |X_{i,j}| \geq 0). \end{aligned}$$

Note that X^2 is diagonal, and that $X = X^1 + X^2$. Because $X_1, X_2 \in \mathrm{cone}\left(\mathcal{B}^n_+ \cup \mathcal{B}^n_-\right)$, we have $X \in \mathrm{cone}\left(\mathcal{B}^n_+ \cup \mathcal{B}^n_-\right)$, and therefore, we get

$$\mathcal{DD}_n \subseteq \mathrm{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-).$$

Conversely, $\forall X \in \mathrm{cone}\left(\mathcal{B}^n_+ \cup \mathcal{B}^n_-\right)$, $\exists \lambda^1_{i,j} \geq 0$ for $1 \leq i \leq j \leq n$ and $\exists \lambda^2_{i,j} \geq 0$ for $1 \leq i < j \leq n$ such that

$$\begin{aligned} X &= \sum_{1 \leq i \leq j \leq n} \lambda^1_{i,j} (e_i + e_j)(e_i + e_j)^T + \sum_{1 \leq i < j \leq n} \lambda^2_{i,j} (e_i - e_j)(e_i - e_j)^T \\ &= \sum_{1 \leq i \leq n} 4\lambda^1_{i,i} e_i e_i^T + \sum_{1 \leq i < j \leq n} \left(\lambda^1_{i,j} (e_i + e_j)(e_i + e_j)^T + \lambda^2_{i,j} (e_i - e_j)(e_i - e_j)^T\right). \end{aligned} \quad (3.3)$$

Note that X is a symmetric matrix. Then from (3.3), we have

$$\forall i < j, \qquad X_{i,j} = \lambda^1_{i,j} - \lambda^2_{i,j}, \tag{3.4}$$

$$\forall i > j, \qquad X_{i,j} = X_{j,i} = \lambda^1_{j,i} - \lambda^2_{j,i}, \tag{3.5}$$

$$\forall i = 1,..,n, \qquad X_{i,i} = 4\lambda^1_{i,i} + \sum_{i<j}(\lambda^1_{i,j} + \lambda^2_{i,j}) + \sum_{i>j}(\lambda^1_{j,i} + \lambda^2_{j,i}). \tag{3.6}$$

Then $\forall i = 1,..,n$,

$$\begin{aligned}
X_{i,i} - \sum_{j \neq i} |X_{i,j}| &= X_{i,i} - \sum_{j>i} |X_{i,j}| - \sum_{j<i} |X_{i,j}| \\
&= X_{i,i} - \sum_{j>i} |\lambda^1_{i,j} - \lambda^2_{i,j}| - \sum_{j<i} |\lambda^1_{j,i} - \lambda^2_{j,i}| \text{ (by (3.4), (3.5))} \\
&\geq X_{i,i} - \sum_{j>i}(|\lambda^1_{i,j}| + |\lambda^2_{i,j}|) - \sum_{j<i}(|\lambda^1_{j,i}| + |\lambda^2_{j,i}|) \text{ (because } |a-b| \leq |a| + |b|) \\
&= X_{i,i} - \sum_{j>i}(\lambda^1_{i,j} + \lambda^2_{i,j}) - \sum_{j<i}(\lambda^1_{j,i} + \lambda^2_{j,i}) \text{ (because } \forall i < j, \lambda^1_{i,j}, \lambda^2_{i,j} \geq 0) \\
&= 4\lambda^1_{i,i} \text{ (By (3.6))} \\
&\geq 0 \text{ (because } \forall i = 1,..,n, \lambda^1_{i,i} \geq 0).
\end{aligned}$$

This implies that X is diagonally dominant, so $X \in \mathcal{DD}_n$, and we get $\text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-) \subseteq \mathcal{DD}_n$. Thus,

$$\text{cone}(\mathcal{B}^n_+ \cup \mathcal{B}^n_-) = \mathcal{DD}_n.$$

□

3.2 An expansion of SD bases and the resulting approximations

When we use SD bases for approximating $\mathcal{S}^n_+$, the sparsity of the matrices in those bases is quite important in terms of computational efficiency. As we mentioned in the last section, for any orthogonal matrix P, $P\mathcal{B}^n_+ P^T$ and $P\mathcal{B}^n_- P^T$ give generalizations of SD bases. However, it is hard to choose an appropriate orthogonal matrix P (except for the identity matrix I) to keep the sparsity of matrices PCP^T and PAP^T in (3.1). In this section, we try to extend the definition of SD bases in order to obtain various sparse SD bases, which will lead us to sparse polyhedral approximations of $\mathcal{S}^n_+$.

In Section 3.2.1, we define the expanded SD basis $\bar{\mathcal{B}}_n(\alpha)$ and the polyhedral approximation based on expanded SD bases: $\mathcal{SDB}_n(\mathcal{H})$. Several essential properties of them are also given. Then in Section 3.2.2, we prove that $\mathcal{SDB}_n(\mathbb{R}) = \mathcal{SDD}_n$, which is the main result of this chapter, and give the inclusive relation among all approximations which are considered in this thesis. Finally in Section 3.2.3, we discuss the choice of parameter set $\mathcal{H}$ when creating polyhedral approximation $\mathcal{SDB}_n(\mathcal{H})$. We give a geometric approach to generate $\mathcal{H}$ that increase the "volume" of $\mathcal{SDB}_n(\mathcal{H})$.

3.2.1 An expansion of SD bases without losing sparsity

We first introduce the definition of expanded SD bases.

Definition 3.2.1. Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere. Define the expansion of the SD basis with one parameter $\alpha \in \mathbb{R}$ as

$$\begin{aligned}\bar{B}_{i,j}(\alpha) &:= (e_i + \alpha e_j)(e_i + \alpha e_j)^T,\\ \bar{\mathcal{B}}_n(\alpha) &:= \{\bar{B}_{i,j}(\alpha) \mid 1 \leq i \leq j \leq n\}.\end{aligned}$$

The proposition below ensures that the expansion of SD bases also gives bases of $\mathbb{S}^n$.

Proposition 3.2.2. Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere. For any $\alpha \in \mathbb{R} \setminus \{0, -1\}$, $\bar{\mathcal{B}}_n(\alpha)$ is a set of $n(n+1)/2$ independent matrices and thus a basis of $\mathbb{S}^n$.

Proof. Let $\alpha \in \mathbb{R} \setminus \{0, -1\}$. Accordingly, for $1 \leq i < j \leq n$, we have

$$\begin{aligned}\bar{B}_{i,j}(\alpha) :=&(e_i + \alpha e_j)(e_i + \alpha e_j)^T\\ =&e_i e_i^T + \alpha(e_i e_j^T + e_j e_i^T) + \alpha^2 e_j e_j^T\\ =&\alpha(e_i e_i^T + e_i e_j^T + e_j e_i^T + e_j e_j^T) + (1-\alpha) e_i e_i^T + (\alpha^2 - \alpha) e_j e_j^T\\ =&\alpha B^+_{i,j} + \frac{1-\alpha}{4} B^+_{i,i} + \frac{\alpha(\alpha-1)}{4} B^+_{j,j},\end{aligned} \tag{3.7}$$

and for every $1 \leq i \leq n$, we also have

$$\begin{aligned}\bar{B}_{i,i}(\alpha) :=&(e_i + \alpha e_i)(e_i + \alpha e_i)^T\\ =&(1+\alpha)^2 e_i e_i^T = \frac{(1+\alpha)^2}{4} B^+_{i,i}.\end{aligned} \tag{3.8}$$

Suppose that there exist $\gamma_{i,j} \geq 0$ $(1 \leq i \leq j \leq n)$ such that

$$\sum_{1 \leq i \leq j \leq n} \gamma_{i,j} \bar{B}_{i,j}(\alpha) = O.$$

Then, by (3.7) and (3.8), we see that

$$
\begin{aligned}
O =& \sum_{i=1}^{n} \frac{\gamma_{i,i}(1+\alpha)^2}{4} B^+_{i,i} + \sum_{1\le i<j\le n} \gamma_{i,j} \left[\alpha B^+_{i,j} + \frac{1-\alpha}{4} B^+_{i,i} + \frac{\alpha(\alpha-1)}{4} B^+_{j,j} \right] \\
=& \sum_{i=1}^{n} \frac{(1+\alpha)^2}{4} \gamma_{i,i} B^+_{i,i} + \sum_{1\le i<j\le n} \alpha\gamma_{i,j} B^+_{i,j} + \sum_{i=1}^{n-1} \frac{1-\alpha}{4} (\sum_{j=i+1}^{n} \gamma_{i,j}) B^+_{i,i} \\
&+ \sum_{j=2}^{n} \frac{\alpha(\alpha-1)}{4} (\sum_{i=1}^{j-1} \gamma_{i,j}) B^+_{j,j} \\
=& \left[\frac{\gamma_{1,1}(1+\alpha)^2}{4} + \frac{1-\alpha}{4} (\sum_{j=2}^{n} \gamma_{1,j}) \right] B^+_{1,1} \\
&+ \sum_{i=2}^{n-1} \left[\frac{(1+\alpha)^2}{4} \gamma_{i,i} + \frac{1-\alpha}{4} (\sum_{j=i+1}^{n} \gamma_{i,j}) + \frac{\alpha(\alpha-1)}{4} (\sum_{j=1}^{i-1} \gamma_{j,i}) \right] B^+_{i,i} \\
&+ \left[\frac{\gamma_{n,n}(1+\alpha)^2}{4} + \frac{\alpha(\alpha-1)}{4} (\sum_{j=1}^{n-1} \gamma_{j,n}) \right] B^+_{n,n} \\
&+ \sum_{1\le i<j\le n} \alpha\gamma_{i,j} B^+_{i,j}.
\end{aligned}
\tag{3.9}
$$

Since $\{B^+_{i,j}\} = \mathcal{B}^n_+$ is a set of linearly independent matrices, all the coefficients for $B_{i,j}$ in (3.9) should be 0. Thus, we have

$$
0 = \frac{\gamma_{1,1}(1+\alpha)^2}{4} + \frac{1-\alpha}{4} (\sum_{j=2}^{n} \gamma_{1,j}), \tag{3.10}
$$

$$
0 = \frac{(1+\alpha)^2}{4} \gamma_{i,i} + \frac{1-\alpha}{4} (\sum_{j=i+1}^{n} \gamma_{i,j}) + \frac{\alpha(\alpha-1)}{4} (\sum_{j=1}^{i-1} \gamma_{j,i}) \ (2 \le i \le n-1), \tag{3.11}
$$

$$
0 = \frac{\gamma_{n,n}(1+\alpha)^2}{4} + \frac{\alpha(\alpha-1)}{4} (\sum_{j=1}^{n-1} \gamma_{j,n}), \tag{3.12}
$$

$$
0 = \alpha\gamma_{i,j} \ (1 \le i < j \le n). \tag{3.13}
$$

Since $\alpha \neq 0$, by (3.13) we have

$$
\gamma_{i,j} = 0 \ (1 \le i < j \le n). \tag{3.14}
$$

Since $\alpha \neq -1$, (3.10)-(3.14) imply that

$$
\gamma_{i,i} = 0 \ (i = 1, 2, \dots, n).
$$

The above leads us to conclude that $\{\bar{B}_{i,j}(\alpha)\} = \bar{\mathcal{B}}_n(\alpha)$ is a set of $n(n+1)/2$ linearly independent matrices. $\square$

If we let $\alpha = 1$, then it is straightforward that $\bar{\mathcal{B}}_n(1) = \mathcal{B}_+^n$. If we let α be other real numbers, we may obtain different SD bases. The following proposition gives the condition for generating different expanded SD bases.

Proposition 3.2.3. *Let $e_i \in \mathbb{R}^n$ denotes the vector with a 1 at the ith coordinate and 0 elsewhere. Suppose that $\alpha_1 \in \mathbb{R} \setminus \{0, -1\}$ and $\alpha_2 \in \mathbb{R} \setminus \{0, \alpha_1\}$. Then, for every $1 \leq i < j \leq n$,*

$$(e_i + \alpha_2 e_j)(e_i + \alpha_2 e_j)^T \notin \mathrm{cone}(\bar{\mathcal{B}}_n(\alpha_1)).$$

Proof. For $1 \leq i \leq j \leq n$, let us define

$$\bar{B}^1_{i,j} := (e_i + \alpha_1 e_j)(e_i + \alpha_1 e_j)^T, \quad \bar{B}^2_{i,j} := (e_i + \alpha_2 e_j)(e_i + \alpha_2 e_j)^T.$$

Note that if $i = j$, then

$$\bar{B}^1_{i,i} := (1 + \alpha_1)^2 e_i e_i^T, \quad \bar{B}^2_{i,i} := (1 + \alpha_2)^2 e_i e_i^T. \tag{3.15}$$

For every $i < j$, we can write $\bar{B}^2_{i,j}$ as a linear combination of $\bar{B}^1_{i,j}$:

$$\begin{aligned}
\bar{B}^2_{i,j} =& e_i e_i^T + \alpha_2^2 e_j e_j^T + \alpha_2(e_i e_j^T + e_j e_i^T) \\
=& e_i e_i^T + \alpha_2^2 e_j e_j^T + \frac{\alpha_2}{\alpha_1}\alpha_1(e_i e_j^T + e_j e_i^T) \quad (\text{because } \alpha_1 \neq 0) \\
=& e_i e_i^T + \alpha_2^2 e_j e_j^T - \frac{\alpha_2}{\alpha_1} e_i e_i^T - \frac{\alpha_2 \alpha_1^2}{\alpha_1} e_j e_j^T \\
&+ \frac{\alpha_2}{\alpha_1}\left[e_i e_i^T + \alpha_1(e_i e_j^T + e_j e_i^T) + \alpha_1^2 e_j e_j^T\right] \\
=& \frac{\alpha_1 - \alpha_2}{\alpha_1} e_i e_i^T + \alpha_2(\alpha_2 - \alpha_1) e_j e_j^T + \frac{\alpha_2}{\alpha_1}\bar{B}^1_{i,j} \\
=& \frac{\alpha_1 - \alpha_2}{\alpha_1(1+\alpha_1)^2}(1+\alpha_1)^2 e_i e_i^T + \frac{\alpha_2(\alpha_2 - \alpha_1)}{(1+\alpha_1)^2}(1+\alpha_1)^2 e_j e_j^T + \frac{\alpha_2}{\alpha_1}\bar{B}^1_{i,j} \\
&(\text{because } \alpha_1 \neq -1) \\
=& \frac{\alpha_1 - \alpha_2}{\alpha_1(1+\alpha_1)^2}\bar{B}^1_{i,i} + \frac{\alpha_2(\alpha_2 - \alpha_1)}{(1+\alpha_1)^2}\bar{B}^1_{j,j} + \frac{\alpha_2}{\alpha_1}\bar{B}^1_{i,j} \text{ (by (3.15))}.
\end{aligned} \tag{3.16}$$

Since $\alpha_1 \notin \{0, -1\}$, Proposition 3.2.2 ensures that $\bar{\mathcal{B}}_n(\alpha_1)$ is linearly independent, and hence, the expression (3.16) for $\bar{B}^2_{i,j}$ is unique.

Suppose that $\bar{B}^2_{i,j} \in \mathrm{cone}\left(\bar{\mathcal{B}}_n(\alpha_1)\right)$. In this case, all the coefficients in (3.16) should be non-negative, which implies that

$$\frac{\alpha_1 - \alpha_2}{\alpha_1(1+\alpha_1)^2} \geq 0,\ \frac{\alpha_2(\alpha_2 - \alpha_1)}{(1+\alpha_1)^2} \geq 0,\ \frac{\alpha_2}{\alpha_1} > 0. \tag{3.17}$$

From the last inequality in (3.17), we have either

$$\text{(i) } \alpha_1, \alpha_2 > 0 \quad \text{or} \quad \text{(ii) } \alpha_1, \alpha_2 < 0.$$

For case (i), from the first and second inequalities of (3.17), we have $\alpha_2 - \alpha_1 \geq 0$ and $\alpha_1 - \alpha_2 \geq 0$, which implies $\alpha_2 = \alpha_1$ and contradicts the assumption $\alpha_2 \neq \alpha_1$. A similar contradiction is obtained for case (ii). Thus, we have $\bar{B}^2_{i,j} \notin \mathrm{cone}(\bar{\mathcal{B}}_n(\alpha_1))$. □

Next we define the inner and outer polyhedral approximations of the semidefinite cone using expanded SD bases.

Definition 3.2.4. Let $\{1, -1\} \subseteq \mathcal{H} \subseteq \mathcal{R}$ be the set of parameters. We define the inner polyhedral approximation of the semidefinite cone using expanded SD bases as

$$\mathcal{SDB}_n(\mathcal{H}) := \mathrm{cone}\left(\bigcup_{\alpha \in \mathcal{H}} \bar{\mathcal{B}}_n(\alpha)\right).$$

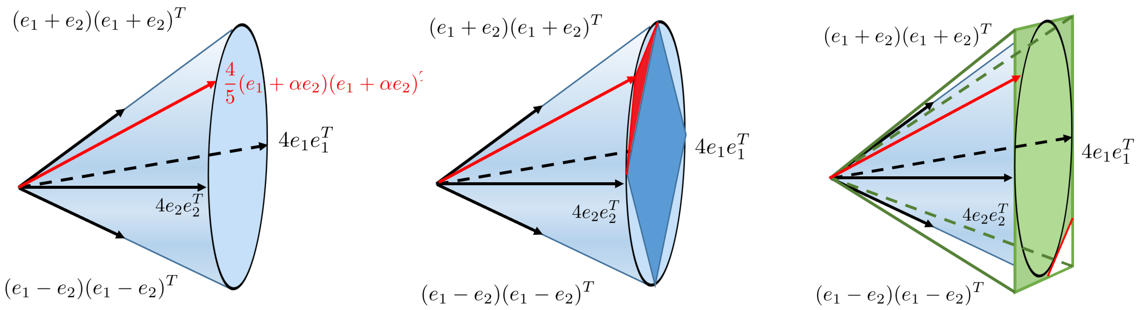
The outer polyhedral approximation of the semidefinite cone is defined as

$$\mathcal{SDB}^*_n(\mathcal{H}) := \{X \in \mathbb{S}^n \mid \langle X, Y \rangle \geq 0,\ \forall Y \in \bar{\mathcal{B}}_n(\alpha),\ \alpha \in \mathcal{H}\}.$$

Example 3.2.5. As an example in $\mathbb{S}^2$, let $e_1 = (1,0)^T$ and $e_2 = (0,1)^T$. Then, in addition to the SD bases of Types I and II listed in Example 3.1.23, we can generate the expanded SD basis with parameter $\alpha = 2$ as

$$\bar{\mathcal{B}}_2(2) = \left\{ \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 9 \end{pmatrix} \right\}.$$

Figure 3.6 [a] shows the intersection between expanded SD basis $\bar{\mathcal{B}}_2(2)$ and hyperplane $\{X \in \mathbb{S}^n \mid \mathrm{Tr}(X) = 4\}$. Similarly, [b] (respectively, [c]) shows the intersection between the same hyperplane and the inner approximation $\mathcal{SDB}_2(\{2\})$ (respectively, outer approximation $\mathcal{SDB}^*_2(\{2\})$) .



[a] $\mathcal{B}_+^2 \cup \mathcal{B}_-^2 \cup \bar{\mathcal{B}}_2(2)$. [b] Inner approximation $\mathcal{SDB}_2(\{2\})$. [c] Outer approximation $\mathcal{SDB}_2^*(\{2\})$.

Figure 3.6: An example of expanded SD bases

We can easily see that $\mathcal{SDB}_n(\{1,-1\})$ is equivalent to $\mathcal{S}_{\text{in}}$ defined in Definition 3.1.24, which is equivalent to $\mathcal{DD}_n$ by Proposition 3.1.28. One can see that for two sets of parameters $\mathcal{H}_1, \mathcal{H}_2$ where $\{1,-1\} \subseteq \mathcal{H}_1 \subseteq \mathcal{H}_2 \subseteq \mathbb{R}$, we have

$$\mathcal{DD}_n \subseteq \mathcal{SDB}_n(\mathcal{H}_1) \subseteq \mathcal{SDB}_n(\mathcal{H}_2) \subseteq \mathcal{S}_+^n. \tag{3.18}$$

3.2.2 An expression of $\mathcal{SDD}_n$ with expanded SD bases

We next give a theorem which shows that the inner approximation defined in Definition 3.2.4 using $\mathbb{R}$ as $\mathcal{H}$ coincides with $\mathcal{FW}_n(2)$ and hence, the set of scaled diagonally dominant matrices $\mathcal{SDD}_n$:

Theorem 3.2.6.

$$\mathcal{SDB}_n(\mathbb{R}) = \mathcal{SDD}_n.$$

Proof. In what follows, we show that

$$\text{cone}\left(\bigcup_{\alpha\in\mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right) = \mathcal{FW}_n(2),$$

where $\mathcal{FW}_n(k)$ is defined in Definition 3.1.3. Then, the assertion of this theorem follows from Lemma 3.1.19.

Let us show that $\mathcal{FW}_n(2) \subseteq \text{cone}\left(\bigcup_{\alpha\in\mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right)$. For any $X \in \mathcal{FW}_n(2)$, there exists a $V \in \mathbb{R}^{n\times m}$ where $X = VV^T$ and each column contains at most 2 non-zero elements. Denote the columns of V as $v_i (i = 1, 2, \ldots, m)$. Here, we can assume that $v_i (i = 1, 2, \ldots, m)$ are non-zero vectors without any loss of generality. Thus, we see that there exist $p(i), q(i) \in$

$\{1, 2, \ldots, n\}(i = 1, 2, \ldots, m)$ and $\alpha_{p(i)}, \alpha_{q(i)} \in \mathbb{R}$, at least either of which is non-zero for every $i = 1, 2, \ldots, m$ satisfying

$$v_i = \alpha_{p(i)} e_{p(i)} + \alpha_{q(i)} e_{q(i)}.$$

For every $i = 1, 2, \ldots, m$, if $\alpha_{p(i)} = 0$, we have

$$v_i v_i^T = \alpha_{q(i)}^2 e_{q(i)} e_{q(i)}^T \in \text{cone}\left(\bigcup_{\alpha \in \mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right), \tag{3.19}$$

and if $\alpha_{p(i)} \neq 0$, we have

$$\begin{aligned} v_i v_i^T =& \alpha_{p(i)}^2 (e_{p(i)} + \frac{\alpha_{q(i)}}{\alpha_{p(i)}} e_{q(i)})(e_{p(i)} + \frac{\alpha_{q(i)}}{\alpha_{p(i)}} e_{q(i)})^T \\ &\in \text{cone}\left(\bigcup_{\alpha \in \mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right). \end{aligned} \tag{3.20}$$

By (3.19) and (3.20), we conclude that

$$X = VV^T = \sum_{i=1}^{m} v_i v_i^T \in \text{cone}\left(\bigcup_{\alpha \in \mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right).$$

Next, we show that $\text{cone}\left(\bigcup_{\alpha \in \mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right) \subseteq \mathcal{FW}_n(2)$.

Suppose that $X \in \text{cone}\left(\bigcup_{\alpha \in \mathbb{R}} \bar{\mathcal{B}}_n(\alpha)\right)$. Then there exist some positive integer k_1 and $\lambda_{ij}^k \geq 0, \alpha^k \in \mathbb{R}$ $(1 \leq i \leq j \leq n,\ 1 \leq k \leq k_1)$ such that

$$\begin{aligned} X &= \sum_{\substack{1 \leq i \leq j \leq n, \\ k=1,..,k_1}} \lambda_{ij}^k (e_i + \alpha^k e_j)(e_i + \alpha^k e_j)^T. \\ &= \sum_{\substack{1 \leq i \leq j \leq n, \\ k=1,..,k_1}} (\sqrt{\lambda_{ij}^k} e_i + \alpha^k \sqrt{\lambda_{ij}^k} e_j)(\sqrt{\lambda_{ij}^k} e_i + \alpha^k \sqrt{\lambda_{ij}^k} e_j)^T. \end{aligned}$$

Define a vector $v(i,j,k) := \sqrt{\lambda_{ij}^k} e_i + \alpha^k \sqrt{\lambda_{ij}^k} e_j$ for any $1 \leq i \leq j \leq n$ and $k \in \{1, .., k_1\}$. Then, $v(i,j,k)$ has at most two nonzero elements, so we can obtain a matrix $V \in \mathbb{R}^{n \times \frac{k_1 n(n+1)}{2}}$ whose columns are $v(i,j,k)$. Then,

$$X = \sum_{\substack{1 \leq i \leq j \leq n, \\ k=1,..,k_1}} v(i,j,k) v(i,j,k)^T = VV^T$$

and by Definition 3.1.3, $X \in \mathcal{FW}_n(2)$. □

By Lemma 3.1.19, we have $\mathcal{SDD}_n = \mathcal{FW}_n(2)$. In addition to the relation between $\mathcal{DD}_n$ and $\mathcal{SDB}_n(\mathcal{H})$ in (3.18), we have the following corollary which shows the inclusive relation among approximations described in this thesis.

Corollary 3.2.7. For any set of parameters $\mathcal{H}:\ \{1,-1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$, we have

$$\mathcal{DD}_n \subseteq \mathcal{SDB}_n(\mathcal{H}) \subseteq \mathcal{SDD}_n = \mathcal{FW}_n(2) \subseteq \ldots \subseteq \mathcal{FW}_n(n) = \mathcal{S}^n_+.$$

Similarly, for outer approximations, we have

$$\mathcal{S}^n_+ = \mathcal{S}^{n,n} \subseteq \ldots \subseteq \mathcal{S}^{n,2} = \mathcal{SDD}^*_n \subseteq \mathcal{SDB}^*_n(\mathcal{H}) \subseteq \mathcal{DD}^*_n.$$

Example 3.2.8. Let I be the identity matrix in $\mathbb{S}^{10}$, and let

$$\bar{\mathcal{H}} = \{\pm 1, \pm 1 \pm \sqrt{2}\}.$$

We use the same matrices $A, B \in \mathbb{S}^{10}$ generated in Example 3.1.4. For given scalars $\alpha, \beta \in \mathbb{R}$, we check whether the matrix $I + \alpha A + \beta B$ is in $\mathcal{DD}_{10}$, $\mathcal{SDD}_{10}$, $\mathcal{SDB}_{10}(\bar{\mathcal{H}})$ and $\mathcal{S}^{10}_+$. Let $\mathcal{G}_{A,B}(\mathcal{S}) := \{(\alpha, \beta) \in \mathbb{R}^2 \mid I + \alpha A + \beta B \in \mathcal{S}\}$. Figure 3.7 shows the region of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{DD}_{10}, \mathcal{SDD}_{10}, \mathcal{SDB}_{10}(\bar{\mathcal{H}}), \mathcal{S}^{10}_+\}$.

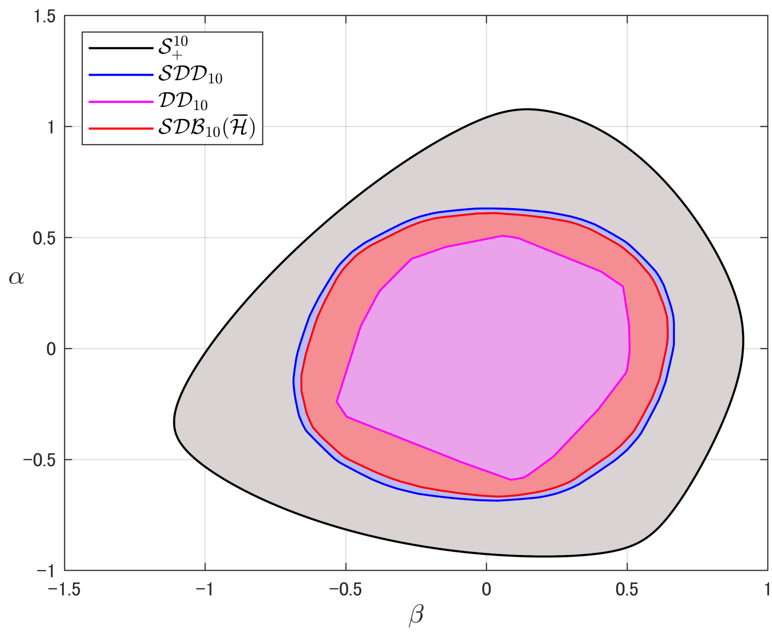


Figure 3.7: Figure of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{DD}_{10}, \mathcal{SDD}_{10}, \mathcal{SDB}_{10}(\bar{\mathcal{H}}), \mathcal{S}^{10}_+\}$.

One can observe that the region of $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\bar{\mathcal{H}}))$ is very close to the region of $\mathcal{G}_{A,B}(\mathcal{SDD}_{10})$.

3.2.3 Notes on choosing the parameter α

Here, we discuss the choice for the parameter α to increase the "volume" of the polyhedral approximation $\mathcal{SDB}_n(\mathcal{H})$ of the semidefinite cone $\mathcal{S}^n_+$. For any $\alpha \in \mathbb{R}$ and $1 \le i < j \le n$, by Definition 3.2.1, we can calculate the Frobenius norm of $\bar{B}_{i,j}(\alpha)$:

$$\begin{aligned}\|\bar{B}_{i,j}(\alpha)\|_F =& \|(e_i + \alpha e_j)(e_i + \alpha e_j)^T\|_F \\ =& \sqrt{\mathrm{Tr}\left((e_i + \alpha e_j)(e_i + \alpha e_j)^T(e_i + \alpha e_j)(e_i + \alpha e_j)^T\right)} \\ =& \|e_i + \alpha e_j\|_2^2 \\ =& 1 + \alpha^2. \end{aligned} \tag{3.21}$$

According to Proposition 3.2.3, by changing α, one can obtain different polyhedral approximations. However, we can see that

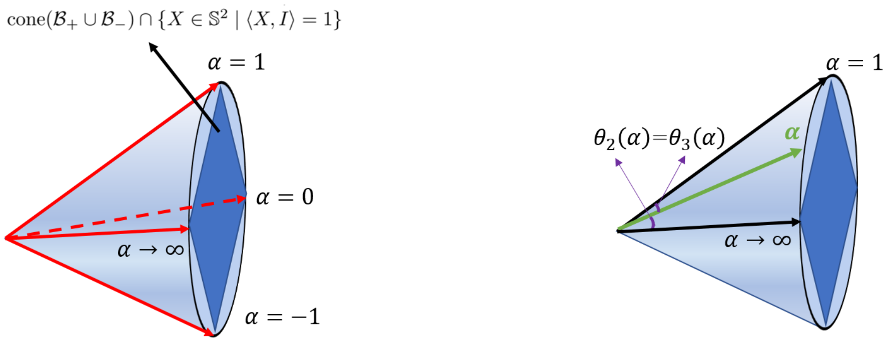
$$\begin{aligned}\lim_{|\alpha|\to\infty} \frac{\bar{B}_{i,j}(\alpha)}{\|\bar{B}_{i,j}(\alpha)\|_F} &= \lim_{|\alpha|\to\infty} \frac{1}{1+\alpha^2}(e_i + \alpha e_j)(e_i + \alpha e_j)^T \text{ (by (3.21))}, \\ &= \lim_{|\alpha|\to\infty} \left[\frac{1}{1+\alpha^2} e_i e_i^T + \frac{\alpha}{1+\alpha^2}(e_i e_j^T + e_j e_i^T) + \frac{\alpha^2}{1+\alpha^2} e_j e_j^T\right] \\ &= e_j e_j^T = \frac{1}{4} B^+_{j,j}, \end{aligned}$$

and by Definitions 3.1.22 and 3.2.1, we have

$$\bar{B}_{i,j}(0) = \frac{1}{4} B^+_{i,i},\ \bar{B}_{i,j}(1) = B^+_{i,j},\ \bar{B}_{i,j}(-1) = B^-_{i,j}.$$

This shows that, if $|\alpha| \to \infty$ or $\alpha \in \{0, 1, -1\}$, the new matrix $\bar{B}_{i,j}(\alpha)$ will become close to the existing matrices, e.g. $B^+_{i,i}$, $B^+_{j,j}$, $B^+_{i,j}$ and $B^-_{i,j}$, and the "volume" of the polyhedral approximation cone$(\bar{\mathcal{B}}_n(\alpha) \cup \mathcal{B}^n_+ \cup \mathcal{B}^n_-)$ of the semidefinite cone $\mathcal{S}^n_+$ will also be close to the "volume" of the existing inner approximation cone$(\mathcal{B}^n_+ \cup \mathcal{B}^n_-)$ of $\mathcal{S}^n_+$.

The red arrow in Fig. 3.8 [a] shows the extreme rays $\{\gamma \bar{B}_{i,j}(\alpha) \mid \gamma \ge 0\}$ with $|\alpha| \to \infty$ and $\alpha \in \{0, 1, -1\}$. The conical hull of these extreme rays is cone$(\mathcal{B}^n_+ \cup \mathcal{B}^n_-)$ and its cross section with $\{X \in \mathbb{S}^2 \mid \langle X, I \rangle = 1\}$ is illustrated as the blue area. To avoid generating a new matrix $\bar{B}_{i,j}(\alpha)$ that is close to the existing matrices, we may choose an α such that the angle between $\bar{B}_{i,j}(\alpha)$ and existing matrices are equal, as illustrated in Fig. 3.8 [b].



[a] The set of $\{\gamma \bar{B}_{i,j}(\alpha) \mid \gamma \geq 0\}$

[b] $\bar{B}_{i,j}(\alpha)$ that are not close to the existing matrices

Figure 3.8: Choice of α to generate $\bar{B}_{i,j}(\alpha) \in \mathbb{S}^2$ in $\mathbb{R}^3$

We expand this idea to the case of generating a matrix $\bar{B}_{i,j}(\alpha) \in \mathbb{S}^n$. Given an $\alpha \in \mathbb{R}$, we can define the angles between matrices in the expanded SD bases and SD bases Type I and II for every $1 \leq i < j \leq n$, as follows:

$$\theta_1(\alpha) := \arccos \frac{\langle \bar{B}_{i,j}(\alpha), B^+_{i,i} \rangle}{\|\bar{B}_{i,j}(\alpha)\|_F \|B^+_{i,i}\|_F}, \ \theta_2(\alpha) := \arccos \frac{\langle \bar{B}_{i,j}(\alpha), B^+_{j,j} \rangle}{\|\bar{B}_{i,j}(\alpha)\|_F \|B^+_{j,j}\|_F},$$
$$\theta_3(\alpha) := \arccos \frac{\langle \bar{B}_{i,j}(\alpha), B^+_{i,j} \rangle}{\|\bar{B}_{i,j}(\alpha)\|_F \|B^+_{i,j}\|_F}, \ \theta_4(\alpha) := \arccos \frac{\langle \bar{B}_{i,j}(\alpha), B^-_{i,j} \rangle}{\|\bar{B}_{i,j}(\alpha)\|_F \|B^-_{i,j}\|_F}.$$

Thus, we have

$$\begin{aligned}
\cos\theta_1(\alpha) &= \frac{\langle \bar{B}_{i,j}(\alpha), B^+_{i,i} \rangle}{\|\bar{B}_{i,j}(\alpha)\|_F \|B^+_{i,i}\|_F} \\
&= \frac{\langle (e_i + \alpha e_j)(e_i + \alpha e_j)^T, (e_i + e_i)(e_i + e_i)^T \rangle}{(1+\alpha^2)\|(e_i + e_i)(e_i + e_i)^T\|_F} \text{ (by (3.21))} \\
&= \frac{4\|e_i\|_2^4}{(1+\alpha^2)4\|e_i\|_2^2} \text{ (because } e_i^T e_j = 0) \\
&= \frac{1}{1+\alpha^2} \text{ (because } \|e_i\|_2 = 1).
\end{aligned}$$

Similarly, we have

$$\cos\theta_2(\alpha) = \frac{\alpha^2}{1+\alpha^2}, \ \cos\theta_3(\alpha) = \frac{(1+\alpha)^2}{2(1+\alpha^2)}, \ \cos\theta_4(\alpha) = \frac{(1-\alpha)^2}{2(1+\alpha^2)}.$$

In general, to obtain a large enough inner approximation with limited parameters, we prefer an α that makes $\theta_1(\alpha) = \theta_3(\alpha)$, which means that the new matrix $\bar{B}_{i,j}(\alpha)$ will be in the middle of $B^+_{i,i}$ and $B^+_{i,j}$ on the boundary of $\mathcal{S}^n_+$. Similarly, we can obtain α by calculating

$\theta_2(\alpha) = \theta_3(\alpha)$, $\theta_1(\alpha) = \theta_4(\alpha)$ and $\theta_2(\alpha) = \theta_4(\alpha)$. By solving these equalities, we find that

$$\alpha = \pm 1 \pm \sqrt{2}.$$

The expansions with these parameters are expected to provide generally large inner approximations for $\mathcal{S}^n_+$.

Example 3.2.9. Let I be the identity matrix in $\mathbb{S}^{10}$, and let

$$\begin{aligned}\bar{\mathcal{H}} =& \{\pm 1, \pm 1 \pm \sqrt{2}\},\\ \mathcal{H}_1 =& \{\pm 1, \pm 100, \pm 0.01\},\\ \mathcal{H}_2 =& \{\pm 1, \pm 5, \pm 0.2\},\end{aligned}$$

We use the same matrices $A, B \in \mathbb{S}^{10}$ generated in Example 3.1.4. For given scalars $\alpha, \beta \in \mathbb{R}$, we check whether the matrix $I + \alpha A + \beta B$ is in $\mathcal{DD}_{10}$, $\mathcal{S}^{10}_+$ and $\mathcal{SDB}_{10}(\mathcal{H})$ with different sets of parameters $\mathcal{H} \in \{\bar{\mathcal{H}}, \mathcal{H}_1, \mathcal{H}_2\}$. Let $\mathcal{G}_{A,B}(\mathcal{S}) := \{(\alpha, \beta) \in \mathbb{R}^2 \mid I + \alpha A + \beta B \in \mathcal{S}\}$. Figure 3.9 shows the region of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{SDB}_{10}(\bar{\mathcal{H}}), \mathcal{SDB}_{10}(\mathcal{H}_1), \mathcal{SDB}_{10}(\mathcal{H}_2), \mathcal{S}^{10}_+\}$.

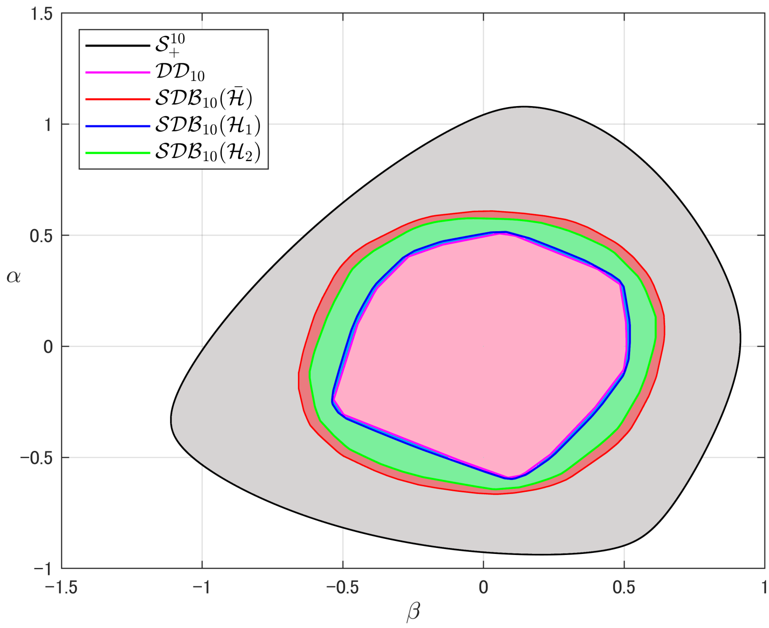


Figure 3.9: Figure of $\mathcal{G}_{A,B}(\mathcal{S})$ where $\mathcal{S} \in \{\mathcal{SDB}_{10}(\bar{\mathcal{H}}), \mathcal{SDB}_{10}(\mathcal{H}_1), \mathcal{SDB}_{10}(\mathcal{H}_2), \mathcal{S}^{10}_+\}$.

As can be seen in the above figure, $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\bar{\mathcal{H}}))$ is the largest among $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\bar{\mathcal{H}}))$, $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\mathcal{H}_1))$ and $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\mathcal{H}_2))$. Also, one can observe that the region of $\mathcal{G}_{A,B}(\mathcal{SDB}_{10}(\mathcal{H}_1))$ is very close to the region of $\mathcal{G}_{A,B}(\mathcal{DD}_{10})$.

3.3 Conclusion

We developed techniques to construct a series of sparse polyhedral approximations of the semidefinite cone. We provided a way to approximate the semidefinite cone using SD bases and proved that the set of diagonally dominant matrices can be expressed with sparse SD bases. A simple expansion of SD bases was proposed, which keeps the sparsity of the matrices that compose it. We gave the conditions for generating linearly independent matrices in expanded SD bases and for generating an expansion different from the existing one. We showed that the polyhedral approximation using our expanded SD bases contains the set of diagonally dominant matrices and is contained in the set of scaled diagonally dominant matrices. The fact that the set of scaled diagonally dominant matrices can be expressed using an infinite number of expanded SD bases was also proved.

Chapter 4

Evaluating approximations of the semidefinite cone

4.1 Introduction

In this chapter, we analyze how well approximations mentioned in Chapter 3 can approximate the semidefinite cone. There are two kinds of approximation, i.e., inner approximation and outer approximation, and an inner approximation (an outer approximation) of $\mathcal{S}^n_+$ can be obtained by constructing the dual cone of an outer approximation (an inner approximation). In practice, the outer approximations are commonly used in cutting-plane methods for solving SDPs (e.g., [1, 2, 17, 114]), and in partial facial reduction techniques for simplifying large-scale SDPs (e.g.,[95]). Note that the computational experiments in Chapter 5 of this thesis use only the outer approximations. Accordingly, we will focus on the outer approximations of $\mathcal{S}^n_+$ and refer to them as approximations of $\mathcal{S}^n_+$ throughout this chapter.

We consider approximations of the semidefinite cone introduced in Chapter 3, including the k-PSD closure, namely $\mathcal{S}^{n,k}$ ([20]) and the dual cone of the set of diagonally dominant matrices (resp., scaled diagonally dominant matrices), namely $\mathcal{DD}^*_n$ (resp., $\mathcal{SDD}^*_n$) ([2]), and the outer approximation using expanded SD bases, namely $\mathcal{SDB}^*_n(\mathcal{H})$ ([114]). Let k and n be positive integers satisfying $2 \le k \le n$, let $\mathcal{H}$ be a set of parameters where $\{1, -1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$, and let

$$\mathcal{S}^{n,k} :=\{X \in \mathbb{S}^n \mid \text{ All } k \times k \text{ principal submatrices of } X \text{ are positive semidefinite}\}. \tag{4.1}$$

$$\mathcal{DD}^*_n :=\{X \in \mathbb{S}^n \mid X_{i,i} + X_{j,j} \pm 2X_{i,j} \ge 0 \ (1 \le i \le j \le n)\}. \tag{4.2}$$

$$\mathcal{SDD}^*_n :=\{X \in \mathbb{S}^n \mid X_{i,i}X_{j,j} \ge X^2_{i,j} \ (1 \le i < j \le n), X_{i,i} \ge 0 \ (i = 1, \dots, n)\}. \tag{4.3}$$

$$\mathcal{SDB}^*_n(\mathcal{H}) :=\{X \in \mathbb{S}^n \mid X_{i,i} + \alpha^2 X_{j,j} + 2\alpha X_{i,j} \ge 0 \ (1 \le i \le j \le n, \ \alpha \in \mathcal{H})\} \tag{4.4}$$

In this chapter, we first show that the norm normalized distance between a set $\mathcal{S}$ and $\mathcal{S}^n_+$ (i.e., the maximum distance from a matrix $X \in \mathcal{S}$ to $\mathcal{S}^n_+$, where the Frobenius norm of the matrix X is assumed to be one) has the same value whenever $\mathcal{SDD}^*_n \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$. This implies that the Frobenius norm constraint may be too strong for the evaluation, and we need a new measure to evaluate these sets. We propose a new measure, the trace normalized distance. We then give the exact values of the trace normalized distance between $\mathcal{DD}^*_n$ and $\mathcal{S}^n_+$ and the distance between $\mathcal{SDD}^*_n$ and $\mathcal{S}^n_+$.

Then, we propose a new measure that evaluates an approximation $\mathcal{S}: \ \mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$ by calculating the the minimum distance from any extreme point of $\mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid \mathrm{Tr}(X) = 1\}$ to the set $\mathcal{S}$, namely the minimum extreme point distance: $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S})$. For each $n \geq 2$, We described how to calculate $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \cdot)$ for approximations $\mathcal{SDB}^*_n(\mathcal{H})$ and $\mathcal{SDD}^*_n$, and give numerical results of these values.

The organization of this chapter is as follows. In Section 4.2, the norm normalized distance proposed by Blekherman et al. [20] is used to evaluate $\mathcal{DD}^*_n$ and $\mathcal{SDD}^*_n$. In Section 4.3, the trace normalized distance is proposed and used to evaluate $\mathcal{DD}^*_n$ and $\mathcal{SDD}^*_n$. In Section 4.4, the minimum extreme point distance $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \cdot)$ is proposed and used to evaluate $\mathcal{SDD}^*_n$ and $\mathcal{SDB}^*_n(\mathcal{H})$ for several different $\mathcal{H}$. We conclude our work in Section 4.5. The contents in Section 4.2 and 4.3 are covered in [115].

4.2 Evaluating approximations of the semidefinite cone with the Frobenius norm normalized distance

Blekherman et al. [20] proposed a method of evaluating approximations of the semidefinite cone, which is based on the maximum distance from a matrix in a given approximation $\mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathbb{S}^n$ to $\mathcal{S}^n_+$. A feature of their method is that the distance is evaluated under the constraint that the value of the Frobenius norm is one, and the norm normalized distance between a set $\mathcal{S}$ and $\mathcal{S}^n_+$ is defined as

$$\overline{\mathrm{dist}}_F(\mathcal{S}, \mathcal{S}^n_+) := \sup_{X \in \mathcal{S}, \|X\|_F = 1} \|X - \mathrm{P}_{\mathcal{S}^n_+}(X)\|_F, \tag{4.5}$$

where $\mathrm{P}_{\mathcal{S}^n_+}(X) := \mathrm{argmin}_{Y \in \mathcal{S}^n_+} \|X - Y\|_F$ is the metric projection of X on $\mathcal{S}^n_+$.

In [20], the authors showed that $\overline{\mathrm{dist}}_F(\mathcal{S}^{n,k}, \mathcal{S}^n_+) \leq \frac{n-k}{n+k-2}$. Through a similar discussion, we can prove the following theorem:

Theorem 4.2.1. For $n \geq 4$,

$$\overline{\mathrm{dist}}_F(\mathcal{DD}^*_n, \mathcal{S}^n_+) = \overline{\mathrm{dist}}_F(\mathcal{SDD}^*_n, \mathcal{S}^n_+) = \frac{n-2}{n}.$$

Proof. We prove the following inequalities:

$$\frac{n-2}{n} \leq \overline{\text{dist}}_F(\mathcal{SDD}_n^*, \mathcal{S}_+^n) \leq \overline{\text{dist}}_F(\mathcal{DD}_n^*, \mathcal{S}_+^n) \leq \frac{n-2}{n}. \tag{4.6}$$

The relation $\mathcal{S}^{n,2} = \mathcal{SDD}_n^*$ in Corollary 3.1.20 implies that

$$\overline{\text{dist}}_F(\mathcal{SDD}_n^*, \mathcal{S}_+^n) = \overline{\text{dist}}_F(\mathcal{S}^{n,2}, \mathcal{S}_+^n).$$

By Theorem 3 in [20], we know that $\overline{\text{dist}}_F(\mathcal{S}^{n,k}, \mathcal{S}_+^n) \geq \frac{n-k}{\sqrt{(k-1)^2 n + n(n-1)}}$ and hence,

$$\overline{\text{dist}}_F(\mathcal{SDD}_n^*, \mathcal{S}_+^n) = \overline{\text{dist}}_F(\mathcal{S}^{n,2}, \mathcal{S}_+^n) \geq \frac{n-2}{\sqrt{(2-1)^2 n + n(n-1)}} = \frac{n-2}{n}. \tag{4.7}$$

The relation $\mathcal{SDD}_n^* \subseteq \mathcal{DD}_n^*$ in Corollary 3.1.20 ensures that

$$\overline{\text{dist}}_F(\mathcal{SDD}_n^*, \mathcal{S}_+^n) \leq \overline{\text{dist}}_F(\mathcal{DD}_n^*, \mathcal{S}_+^n). \tag{4.8}$$

Next, we prove that $\overline{\text{dist}}_F(\mathcal{DD}_n^*, \mathcal{S}_+^n) \leq \frac{n-2}{n}$ with the following idea. If a scalar U satisfies $\|X - \text{P}_{\mathcal{S}_+^n}(X)\|_F \leq U$ for every $X \in \mathcal{DD}_n^*$ with $\|X\|_F = 1$, then U is an upper bound on $\overline{\text{dist}}_F(\mathcal{DD}_n^*, \mathcal{S}_+^n)$. We can find such a scalar U by constructing a matrix $\tilde{X} \in \mathcal{S}_+^n$ and a scalar $\tilde{\alpha} \geq 0$ for every $X \in \mathcal{DD}_n^*$ with $\|X\|_F = 1$ so that $\|X - \text{P}_{\mathcal{S}_+^n}(X)\|_F \leq \|X - \tilde{\alpha}\tilde{X}\|_F$.

Let X be a matrix in $\mathcal{DD}_n^*$ satisfying $\|X\|_F = 1$. Define a matrix $X^{(i,j)} \in \mathbb{S}^n$ for every $1 \leq i < j \leq n$:

$$X_{p,q}^{(i,j)} := \begin{cases} \frac{X_{i,i}+X_{j,j}}{2} & (\text{if } p = q \in \{i,j\}), \\ X_{i,j} & (\text{if } (p,q) \in \{(i,j),(j,i)\}), \\ 0 & (\text{otherwise}). \end{cases} \tag{4.9}$$

Let $C_n^k := \frac{n!}{(n-k)!k!}$ and let $\bar{X} := \frac{1}{C_n^2}\sum_{1 \leq i < j \leq n} X^{(i,j)}$. By definitions (4.2) and (4.9), one can verify that $X^{(i,j)} \in \mathcal{S}_+^n$ for all $1 \leq i < j \leq n$, and hence $\bar{X} \in \mathcal{S}_+^n$. Let α be a scalar satisfying $\alpha \geq \frac{2n(n-1)}{3n-4} > 0$. For all $1 \leq i < j \leq n$, we can obtain from (4.9) that $\bar{X}_{i,j} = \bar{X}_{j,i} = \frac{1}{C_n^2} X_{i,j}$ and hence,

$$\sum_{i \neq j}(X_{i,j} - \alpha\bar{X}_{i,j})^2 = \sum_{i \neq j}(1 - \frac{\alpha}{C_n^2})^2 X_{i,j}^2. \tag{4.10}$$

For all $i = 1, \dots, n$, (4.9) implies that $\bar{X}_{i,i} = \frac{1}{C_n^2}\left(\frac{n-2}{2}X_{i,i} + \frac{1}{2}\mathrm{Tr}(X)\right)$ and hence,

$$\begin{aligned}
\sum_{i=1}^{n}(X_{i,i} - \alpha\bar{X}_{i,i})^2 =& \sum_{i=1}^{n}((1 - \frac{\alpha(n-2)}{2C_n^2})X_{i,i} - \frac{\alpha}{2C_n^2}\mathrm{Tr}(X))^2 \\
=& \sum_{i=1}^{n}((1 - \frac{\alpha(n-2)}{2C_n^2})^2 X_{i,i}^2 - 2(1 - \frac{\alpha(n-2)}{2C_n^2})X_{i,i}\frac{\alpha}{2C_n^2}\mathrm{Tr}(X) \\
&+ \frac{\alpha^2}{4(C_n^2)^2}\mathrm{Tr}(X)^2) \\
=&(1 - \frac{\alpha(n-2)}{2C_n^2})^2\sum_{i=1}^{n}X_{i,i}^2 - (\frac{\alpha}{C_n^2} - \frac{\alpha^2(n-2)}{2(C_n^2)^2})\mathrm{Tr}(X)\sum_{i=1}^{n}X_{i,i} \\
&+ \frac{\alpha^2 n}{4(C_n^2)^2}\mathrm{Tr}(X)^2 \\
=&(1 - \frac{\alpha(n-2)}{2C_n^2})^2\sum_{i=1}^{n}X_{i,i}^2 + (\frac{\alpha^2(3n-4)}{4(C_n^2)^2} - \frac{\alpha}{C_n^2})\mathrm{Tr}(X)^2. \qquad (4.11)
\end{aligned}$$

The assumption $\alpha \geq \frac{2n(n-1)}{3n-4}$ ensures that $\frac{\alpha^2(3n-4)}{4(C_n^2)^2} - \frac{\alpha}{C_n^2} \geq 0$. One can verify that $\mathrm{Tr}(X)^2 \leq n\sum_{i=1}^{n}X_{i,i}^2$ by using Cauchy-Schwarz inequality. Then, it follows from (4.11) that

$$\begin{aligned}
\sum_{i=1}^{n}(X_{i,i} - \alpha\bar{X}_{i,i})^2 \leq&(1 - \frac{\alpha(n-2)}{2C_n^2})^2\sum_{i=1}^{n}X_{i,i}^2 + (\frac{\alpha^2(3n-4)}{4(C_n^2)^2} - \frac{\alpha}{C_n^2})n\sum_{i=1}^{n}X_{i,i}^2 \\
=&\left((1 - \frac{\alpha(n-2)}{2C_n^2})^2 + \frac{\alpha^2 n(3n-4)}{4(C_n^2)^2} - \frac{\alpha n}{C_n^2}\right)\sum_{i=1}^{n}X_{i,i}^2 \\
=&\left(1 - \frac{2\alpha(n-2)}{2C_n^2} + \frac{\alpha^2(n-2)^2}{4(C_n^2)^2} + \frac{\alpha^2 n(3n-4)}{4(C_n^2)^2} - \frac{\alpha n}{C_n^2}\right)\sum_{i=1}^{n}X_{i,i}^2 \\
=&\left(1 - \frac{\alpha(n-2+n)}{C_n^2} + \frac{\alpha^2(n^2-4n+4+3n^2-4n)}{4(C_n^2)^2}\right)\sum_{i=1}^{n}X_{i,i}^2 \\
=&\left(1 - \frac{2\alpha(n-1)}{C_n^2} + \frac{4\alpha^2(n-1)^2}{4(C_n^2)^2}\right)\sum_{i=1}^{n}X_{i,i}^2 \\
=&\left(1 - \frac{\alpha(n-1)}{C_n^2}\right)^2\sum_{i=1}^{n}X_{i,i}^2. \qquad (4.12)
\end{aligned}$$

Combining (4.10) and (4.12) gives

$$\|X - \alpha\bar{X}\|_F \leq \sqrt{\sum_{i\neq j}(1 - \frac{\alpha}{C_n^2})^2 X_{i,j}^2 + \left(1 - \frac{\alpha(n-1)}{C_n^2}\right)^2\sum_{i=1}^{n}X_{i,i}^2}. \qquad (4.13)$$

Note that $\bar{\alpha} := n-1$ satisfies $\bar{\alpha} \geq \frac{2n(n-1)}{3n-4}$ when $n \geq 4$, and the coefficients in (4.13) satisfy

$$1 - \frac{\bar{\alpha}}{C_n^2} = -(1 - \frac{\bar{\alpha}(n-1)}{C_n^2}) = \frac{n-2}{n}.$$

Since $\|X\|_F = 1$, by substituting $\bar{\alpha}$ into (4.13), we have

$$\begin{aligned} \|X - \bar{\alpha}\bar{X}\|_F \leq & \sqrt{\left(\frac{n-2}{n}\right)^2 \sum_{i \neq j} X_{i,j}^2 + \left(\frac{n-2}{n}\right)^2 \sum_{i=1}^{n} X_{i,i}^2} \\ = & \frac{n-2}{n} \|X\|_F^2 \\ = & \frac{n-2}{n}. \end{aligned}$$

Because $\bar{X} \in \mathcal{S}_+^n$ and $\bar{\alpha} \geq 0$, by letting $U = \frac{n-2}{n}$, we have

$$\|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F \leq \|X - \bar{\alpha}\bar{X}\|_F \leq U = \frac{n-2}{n}$$

and hence,

$$\overline{\mathrm{dist}}_F(\mathcal{DD}_n^*, \mathcal{S}_+^n) = \sup_{X \in \mathcal{DD}_n^*, \|X\|_F = 1} \|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F \leq U = \frac{n-2}{n}. \tag{4.14}$$

(4.7), (4.8) and (4.14) imply that (4.6) holds, which proves this theorem.

□

Theorem 4.2.1 shows unfortunately that the norm normalized distance (4.5) gives the same value $\overline{\mathrm{dist}}_F(\mathcal{S}, \mathcal{S}_+^n) = \frac{n-2}{n}$ for any approximation $\mathcal{S} \subseteq \mathbb{S}^n$ whenever it satisfies $\mathcal{SDD}_n^* \subseteq \mathcal{S} \subseteq \mathcal{DD}_n^*$. In the next section, we introduce a new distance, called the trace normalized distance. We show that the new distance between $\mathcal{SDD}_n^*$ and $\mathcal{S}_+^n$ has a different value from the one between $\mathcal{DD}_n^*$ and $\mathcal{S}_+^n$.

4.3 Evaluating approximations of the semidefinite cone with the trace normalized distance

The Frobenius norm normalized distance can be generalized by expanding the normalization method and the distance function. For example, let $f : \mathbb{S}^n \to \mathbb{R}$ be a normalization function, and let $p \in [1, \infty)$. One can define the $(f(\cdot), p)$ distance from $\mathcal{S}$ to $\mathcal{S}_+^n$ as:

$$\overline{\mathrm{dist}}_{(f(\cdot),p)}(\mathcal{S}, \mathcal{S}_+^n) := \sup_{X \in \mathcal{S}, f(X)=1} \|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_p, \tag{4.15}$$

where $\|X\|_p := \sqrt[p]{\sum_{i=1}^n |\lambda_i|^p}$, where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of X, denotes the Schatten p-norm of $X \in \mathbb{S}^n$. In this notation, the Frobenius norm normalized distance (4.5) can be rewritten as an $(\|\cdot\|_F, 2)$ distance (4.15).

Recently, Blekherman et al. [21] studied a hyperbolic relaxation of $\mathcal{S}^{n,k}$ and provided an upper bound on the $(f(\cdot), \infty)$ distance from $\mathcal{S}^{n,k}$ to $\mathcal{S}^n_+$, where f can be any unitarily invariant matrix norm or the trace function. In this section, instead of evaluating the most negative eigenvalue of the matrices in the approximation $\mathcal{S}$, we try to figure out how $\mathcal{S}$ approximates $\mathcal{S}^n_+$ from a geometric point of view; i.e., we set $p = 2$ and stick with the Euclidean norm $\|\cdot\|_F$ of $\mathbb{S}^n$.

One reason why the Frobenius normalized distance (4.5) fails to distinguish $\mathcal{DD}^*_n$ and $\mathcal{SDD}^*_n$ might be that the constraint $\|X\|_F = 1$ is restrictive and makes the set $\{X \in \mathbb{S}^n \mid \|X\|_F = 1\}$ bounded. The required properties for normalization methods (e.g., $f(\cdot)$) here are only to make $\{X \in \mathcal{DD}^*_n \mid f(X) = 1\}$ and $\{X \in \mathcal{SDD}^*_n \mid f(X) = 1\}$ bounded.

There are some choices of the normalization method. For example, one may consider bounding another norm (i.e., $\|X\| = 1$), the determinant (i.e., $|X| = 1$), or the trace (i.e., $\mathrm{Tr}(X) := \sum_{i=1}^n X_{i,i} = 1$) of all matrices $X \in \mathbb{S}^n$.

In the case of using other norms, we know from the equivalence of norms (e.g., Corollary 5.4.5 [59]) that for any norm $\|\cdot\|$ on $\mathbb{S}^n$, there exists finite positive constants C_m and C_M such that for all $X \in \mathbb{S}^n$,

$$C_m\|X\| \leq \|X\|_F \leq C_M\|X\|.$$

This implies that for any given norm $\|\cdot\|$ on $\mathbb{S}^n$, the set $\{X \in \mathbb{S}^n \mid \|X\| = 1\}$ itself is also compact (e.g., Corollary 5.4.8 [59]).

As for the choice of determinant, although $\{X \in \mathbb{S}^n \mid |X| = 1\}$ is unbounded, one may notice from a simple example that $\mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid |X| = 1\}$ is unbounded. This implies that the determinant is not adequate to be used for normalizing $\mathcal{DD}^*_n$.

Example 4.3.1. Consider a matrix $X \in \mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid |X| = 1\}$, defined by

$$X := \begin{pmatrix} I & & \\ & \sqrt{x^2+1} & x \\ & x & \sqrt{x^2+1} \end{pmatrix},$$

where I is the $(n-2) \times (n-2)$ identity matrix, and $x \in \mathbb{R} \setminus \{0\}$. It is easy to verify that $|X| = 1$ and $X \in \mathcal{DD}^*_n$, while $\|X\|_F$ can take an arbitrarily large value.

Similarly, $\{X \in \mathbb{S}^n \mid \mathrm{Tr}(X) = 1\}$ is unbounded but one can show that $\{X \in \mathcal{DD}^*_n \mid$

$\mathrm{Tr}(X) = 1\}$ and $\{X \in \mathcal{SDD}_n^* \mid \mathrm{Tr}(X) = 1\}$ are both bounded. Note as well that since $\mathrm{Tr}(X) = 1$ is a linear constraint, the subset of the polyhedral cone $\mathcal{DD}_n^*$ with trace equal to 1, i.e., $\{X \in \mathcal{DD}_n^* \mid \mathrm{Tr}(X) = 1\}$, is still polyhedral. In fact, we used this fact to derive the trace normalized distance between $\mathcal{DD}_n^*$ and $\mathcal{S}_+^n$. From the above discussion, we consider that a distance using the trace is effective for identifying the sets $\mathcal{DD}_n^*$ and $\mathcal{SDD}_n^*$.

Remark 4.3.2. There actually is a very interesting norm which can be seen as a normalization method equivalent to $\mathrm{Tr}(\cdot)$ on $\mathcal{DD}_n^*$ and $\mathcal{SDD}_n^*$. Let $\mathcal{K}$ be a regular cone (i.e., $\mathcal{K}$ is convex closed pointed with nonempty interior) where $I \in \mathrm{int}K^*$, and $\|X\|_I := \min\{\mathrm{Tr}(X_1 + X_2) \mid X_1 - X_2 = X,\ X_1, X_2 \in \mathcal{K}\}$ be the norm induced by I, which was introduced in [44]. Proposition 1 of [44] implies that $\|X\|_I = \mathrm{Tr}(X)$ if $X \in \mathcal{K}$. By letting $\mathcal{K} = \mathcal{DD}_n^*$, it is straightforward that $\{X \in \mathcal{DD}_n^* \mid \|X\|_I = 1\} = \{X \in \mathcal{DD}_n^* \mid \mathrm{Tr}(X) = 1\}$. Since $\mathcal{SDD}_n^* \subseteq \mathcal{DD}_n^*$, $\|\cdot\|_I$ and $\mathrm{Tr}(\cdot)$ are also equivalent on $\mathcal{SDD}_n^*$.

We are now ready to use the Frobenius norm as the distance function and the trace function as the normalization method in (4.15). To simplify the notation, we will rewrite the $(\mathrm{Tr}(\cdot), 2)$ distance (4.15) into the following trace normalized distance from a set $\mathcal{S}$ and $\mathcal{S}_+^n$:

$$\overline{\mathrm{dist}}_T(\mathcal{S}, \mathcal{S}_+^n) := \sup_{X \in \mathcal{S}, \mathrm{Tr}(X)=1} \|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F. \tag{4.16}$$

As shown in the sections below, $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$ and $\overline{\mathrm{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$ are different, i.e., $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n) = \frac{n-2}{n}$ (Theorem 4.3.3) and $\overline{\mathrm{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n) = \frac{\sqrt{n}-1}{2}$ (Theorem 4.3.6).

Figure 4.1 shows the trace normalized distances $\overline{\mathrm{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$ and $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$ with $n = 2, \ldots, 50$.

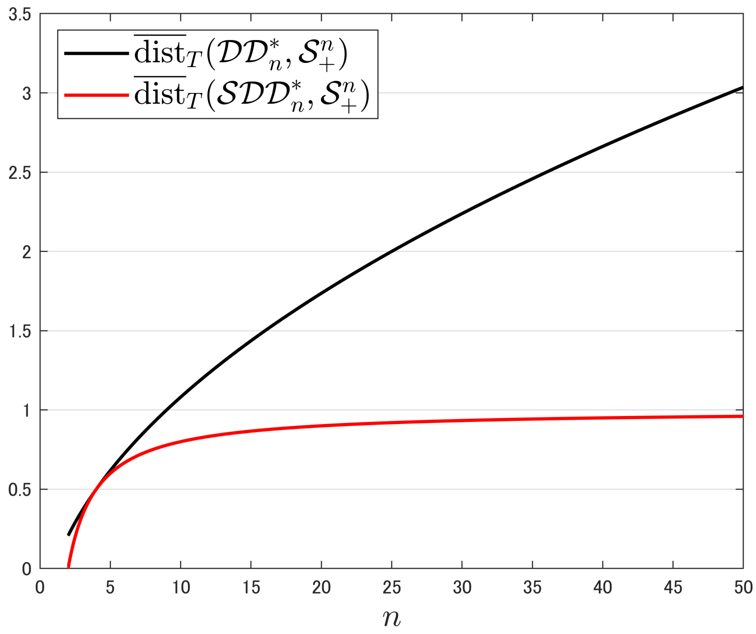


Figure 4.1: The trace normalized distances $\overline{\mathrm{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$ and $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$.

4.3.1 The trace normalized distance between $\mathcal{SDD}_n^*$ and $\mathcal{S}_+^n$

Theorem 4.3.3. For all $n \geq 2$,

$$\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n) = \frac{n-2}{n}.$$

To prove this theorem, we introduce Lemmas 4.3.4 and 4.3.5. Lemma 4.3.4 gives a lower bound on $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$ and Lemma 4.3.5 gives an upper bound on $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$. In these lemmas, we assume that $n \geq 3$. If $n = 2$, we can easily see that $\overline{\mathrm{dist}}_T(\mathcal{SDD}_2^*, \mathcal{S}_+^2) = \overline{\mathrm{dist}}_T(\mathcal{S}_+^2, \mathcal{S}_+^2) = \frac{n-2}{n} = 0$.

Lemmas 4.3.4 and 4.3.5 are based on the results shown in the proofs of Theorems 3 and 1 in [20].

Lemma 4.3.4. For all $n \geq 3$,

$$\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n) \geq \frac{n-2}{n}.$$

Proof. Let $I \in \mathbb{S}^n$ be the identity matrix and $e := (1, \dots, 1)^T \in \mathbb{R}^n$. Given scalars $a, b \geq 0$, we define a matrix,

$$G(a, b, n) := (a+b)I - aee^T. \tag{4.17}$$

If $G(a,b,n) \in \mathcal{SDD}_n^* \setminus \mathcal{S}_+^n$ and $\mathrm{Tr}(G(a,b,n)) = 1$, then by definition (4.16), $\|G(a,b,n) - \mathrm{P}_{\mathcal{S}_+^n}(G(a,b,n))\|_F$ gives a lower bound on $\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n)$. To find a tighter lower bound, we consider the following problem (4.18) on the parameters a and b:

$$\begin{aligned} \max_{a,b\geq 0} \quad & \|G(a,b,n) - \mathrm{P}_{\mathcal{S}_+^n}(G(a,b,n))\|_F && \text{(4.18a)} \\ \text{s.t.} \quad & G(a,b,n) \notin \mathcal{S}_+^n, && \text{(4.18b)} \\ & G(a,b,n) \in \mathcal{SDD}_n^*, && \text{(4.18c)} \\ & \mathrm{Tr}(G(a,b,n)) = 1. && \text{(4.18d)} \end{aligned}$$

Problem (4.18) can be equivalently written as problem (4.19):

$$\begin{aligned} \max_{a,b\geq 0} \quad & (n-1)a - b && \text{(4.19a)} \\ \text{s.t.} \quad & b < (n-1)a, && \text{(4.19b)} \\ & b \geq a, && \text{(4.19c)} \\ & nb = 1. && \text{(4.19d)} \end{aligned}$$

To prove the equivalence between (4.18) and (4.19), we first show that the constraints (4.18b) and (4.19b) are equivalent. Proposition 4 in [20] ensures that the eigenvalues of $G(a,b,n)$ are $a+b$ with multiplicity $n-1$ and $b-(n-1)a$ with multiplicity 1. Note that $a,b \geq 0$; hence,

$$G(a,b,n) \notin \mathcal{S}_+^n \text{ if and only if } b < (n-1)a. \tag{4.20}$$

Next, we verify that (4.18c) and (4.19c) are equivalent. It follows from definition (4.3) that $G(a,b,n) \in \mathcal{SDD}_n^*$ if and only if all the 2×2 submatrices of $G(a,b,n)$ are positive semidefinite. It is obvious from (4.17) that any 2×2 submatrix of $G(a,b,n)$ is $G(a,b,2)$. (4.20) ensures that $G(a,b,2) \in \mathcal{S}_+^2$ if and only if $b \geq a$ and we can conclude that

$$G(a,b,n) \in \mathcal{SDD}_n^* \text{ if and only if } b \geq a. \tag{4.21}$$

The equivalence between (4.18d) and (4.19d) comes from the fact that the definition (4.17) implies that

$$\mathrm{Tr}(G(a,b,n)) = nb. \tag{4.22}$$

We finally show that the objective functions (4.18a) and (4.19a) are equivalent. Since (4.18b) implies that $G(a,b,n) \notin \mathcal{S}_+^n$, it is apparent from (4.20) that $b-(n-1)a < 0$. Then,

$b-(n-1)a$ is the only negative eigenvalue of $G(a,b,n)$, and hence,

$$\|G(a,b,n) - \mathrm{P}_{\mathcal{S}^n_+}(G(a,b,n))\|_F = (n-1)a - b. \tag{4.23}$$

By (4.20), (4.21), (4.22) and (4.23), one can see that problems (4.18) and (4.19) are equivalent. The optimal solution of problem (4.19) is $\bar{a} = \bar{b} = \frac{1}{n}$; hence, we have

$$\overline{\mathrm{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+) \geq \|G(\bar{a}, \bar{b}, n) - \mathrm{P}_{\mathcal{S}^n_+}(G(\bar{a}, \bar{b}, n))\|_F = \frac{n-2}{n}.$$

□

Lemma 4.3.5. For all $n \geq 3$,

$$\overline{\mathrm{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+) \leq \frac{n-2}{n}.$$

Proof. If a scalar U satisfies $\|X - \mathrm{P}_{\mathcal{S}^n_+}(X)\|_F \leq U$ for every $X \in \mathcal{SDD}^*_n$ with $\mathrm{Tr}(X) = 1$, then U is an upper bound on $\overline{\mathrm{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+)$. Below, we find such a scalar U.

Let X be a matrix in $\mathcal{SDD}^*_n$ satisfying $\mathrm{Tr}(X) = 1$. We construct a matrix $\tilde{X} \in \mathcal{S}^n_+$ and a scalar $\tilde{\alpha} \geq 0$ so that $\|X - \mathrm{P}_{\mathcal{S}^n_+}(X)\|_F \leq \|X - \tilde{\alpha}\tilde{X}\|_F$.

Define a matrix $X^{(i,j)} \in \mathbb{S}^n$ for every $1 \leq i < j \leq n$:

$$X^{(i,j)}_{p,q} := \begin{cases} X_{i,i} & (\text{if } p = q = i), \\ X_{j,j} & (\text{if } p = q = j), \\ X_{i,j} & (\text{if } (p,q) \in \{(i,j),(j,i)\}), \\ 0 & (\text{otherwise}). \end{cases} \tag{4.24}$$

Let $\tilde{X} = \frac{1}{C^2_n} \sum_{1 \leq i < j \leq n} X^{(i,j)}$. Then (4.24) implies that

$$\begin{aligned} \tilde{X}_{i,i} &= \frac{C^2_n - C^2_{n-1}}{C^2_n} X_{i,i} = \frac{2}{n} X_{i,i} \ (i = 1, \ldots, n), \\ \tilde{X}_{i,j} &= \frac{1}{C^2_n} X_{i,j} = \frac{2}{n(n-1)} X_{i,j} \ (1 \leq i < j \leq n). \end{aligned}$$

By (4.3), we know that $X^{(i,j)} \in \mathcal{S}^n_+$ for all $1 \leq i < j \leq n$ and hence $\tilde{X} \in \mathcal{S}^n_+$.

Let α be a scalar satisfying $\alpha \geq 0$. Then,

$$
\begin{aligned}
\|X - \alpha\tilde{X}\| &= \sqrt{\sum_{i=1}^{n}(X - \alpha\tilde{X})_{i,i}^2 + \sum_{i\neq j}(X - \alpha\tilde{X})_{i,j}^2} \\
&= \sqrt{\sum_{i=1}^{n}(1 - \frac{2\alpha}{n})^2 X_{i,i}^2 + \sum_{i\neq j}(1 - \frac{2\alpha}{n(n-1)})^2 X_{i,j}^2} \\
&\leq \sqrt{(1 - \frac{2\alpha}{n})^2 \sum_{i=1}^{n} X_{i,i}^2 + (1 - \frac{2\alpha}{n(n-1)})^2 \sum_{i\neq j} X_{i,i}X_{j,j}} \\
&= \sqrt{(1 - \frac{2\alpha}{n})^2 \sum_{i=1}^{n} X_{i,i}^2 + (1 - \frac{2\alpha}{n(n-1)})^2 (\mathrm{Tr}(X)^2 - \sum_{i=1}^{n} X_{i,i}^2)} \\
&= \sqrt{\left((1 - \frac{2\alpha}{n})^2 - (1 - \frac{2\alpha}{n(n-1)})^2\right) \sum_{i=1}^{n} X_{i,i}^2 + (1 - \frac{2\alpha}{n(n-1)})^2 \mathrm{Tr}(X)^2} \\
&= \sqrt{\left(1 - \frac{4\alpha}{n} + \frac{4\alpha^2}{n^2} - (1 - \frac{4\alpha}{n(n-1)} + \frac{4\alpha^2}{n^2(n-1)^2})\right) \sum_{i=1}^{n} X_{i,i}^2 + (1 - \frac{2\alpha}{n(n-1)})^2 \mathrm{Tr}(X)^2} \\
&= \sqrt{\left(\frac{4\alpha^2(n-2)}{n(n-1)^2} - \frac{4\alpha(n-2)}{n(n-1)}\right) \sum_{i=1}^{n} X_{i,i}^2 + (1 - \frac{2\alpha}{n(n-1)})^2 \mathrm{Tr}(X)^2}. \qquad (4.25)
\end{aligned}
$$

Note that $\mathrm{Tr}(X) = 1$ and $\tilde{\alpha} := n - 1 \geq 0$ satisfies that $\frac{4\tilde{\alpha}^2(n-2)}{n(n-1)^2} - \frac{4\tilde{\alpha}(n-2)}{n(n-1)} = 0$. By substituting $\tilde{\alpha}$ into (4.25), we have

$$
\|X - \tilde{\alpha}\tilde{X}\|_F \leq \sqrt{(1 - \frac{2\tilde{\alpha}}{n(n-1)})^2} = \frac{n-2}{n}.
$$

Since $\tilde{\alpha} \geq 0$ and $\tilde{X} \in \mathcal{S}_+^n$, by letting $U = \frac{n-2}{n}$, we can see that

$$
\|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F \leq \|X - \tilde{\alpha}\tilde{X}\|_F \leq U = \frac{n-2}{n},
$$

and hence,

$$
\overline{\mathrm{dist}}_T(\mathcal{SDD}_n^*, \mathcal{S}_+^n) = \sup_{X \in \mathcal{SDD}_n^*, \mathrm{Tr}(X)=1} \|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F \leq U = \frac{n-2}{n}.
$$

□

4.3.2 The trace normalized distance between $\mathcal{DD}_n^*$ and $\mathcal{S}_+^n$

In this section, we prove the following theorem:

Theorem 4.3.6. For all $n \geq 2$,

$$\overline{\text{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n) = \frac{\sqrt{n}-1}{2}.$$

As a corollary of Theorems 4.3.3 and 4.3.6, we obtain an upper bound and a lower bound for $\overline{\text{dist}}_T(\mathcal{SDB}_n^*(\mathcal{H}), \mathcal{S}_+^n)$, where $\{1, -1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$.

Corollary 4.3.7. For $n \geq 2$ and for any set of parameters $\mathcal{H} \subseteq \mathbb{R}$ where $\{1, -1\} \subseteq \mathcal{H}$, we have

$$\frac{n-2}{n} \leq \overline{\text{dist}}_T(\mathcal{SDB}_n^*(\mathcal{H}), \mathcal{S}_+^n) \leq \frac{\sqrt{n}-1}{2}.$$

The idea for proving Theorem 4.3.6 is as follows. Define

$$\mathcal{DDT}_n^* := \mathcal{DD}_n^* \cap \{X \in \mathbb{S}^n \mid \text{Tr}(X) = 1\}. \tag{4.26}$$

Definition (4.16) ensures that

$$\overline{\text{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n) = \max_{X \in \mathcal{DDT}_n^*} \|X - \text{P}_{\mathcal{S}_+^n}(X)\|_F.$$

Note that $\|X - \text{P}_{\mathcal{S}_+^n}(X)\|_F$ is continuous and convex on $\mathbb{S}^n$, and $\mathcal{DDT}_n^*$ is closed, bounded, and convex. Recall that the Bauer maximum principle [11] states that any continuous convex function defined on a compact convex set in $\mathbb{R}^n$ attains its maximum at some extreme point of the set. As its corollary, we have the following result:

Corollary 4.3.8. $\max_{X \in \mathcal{DDT}_n^*} \|X - \text{P}_{\mathcal{S}_+^n}(X)\|_F$ attains its maximum at some extreme point of $\mathcal{DDT}_n^*$.

In Proposition 4.3.9, we show that every extreme point of $\mathcal{DDT}_n^*$ has a special structure. By using this special structure, Lemma 4.3.10 shows that for each extreme point of $\mathcal{DDT}_n^*$, the distance from it to $\mathcal{S}_+^n$ is the same. The exact value of this distance is also given in Lemma 4.3.10. Theorem 4.3.6 can be obtained as a direct result of Corollary 4.3.8 and Lemma 4.3.10.

Proposition 4.3.9. For $n \geq 2$, let X be an extreme point of $\mathcal{DDT}_n^*$. There exists an integer q satisfying $1 \le q \le n$ such that

$$X_{i,j} = \begin{cases} 1 & (\text{ if } i = j = q), \\ \frac{1}{2} \text{ or } -\frac{1}{2} & (\text{ if either } i = q \text{ or } j = q), \\ 0 & (\text{ otherwise}). \end{cases} \tag{4.27}$$

Proof. Let $X \in \mathcal{DDT}_n^*$. By (4.2) and (4.26), we see that for every $i = 1, \dots, n$,

$$X_{i,i} \ge 0,$$

and for every $1 \le i < j \le n$,

$$X_{i,i} + X_{j,j} + 2X_{i,j} \ge 0, \tag{4.28}$$

$$X_{i,i} + X_{j,j} - 2X_{i,j} \ge 0. \tag{4.29}$$

Thus, the set $\mathcal{DDT}_n^*$ can be written as

$$\begin{aligned} \mathcal{DDT}_n^* = \{X \in \mathbb{S}^n \mid & \mathrm{Tr}(X) = 1, \\ & X_{i,i} \ge 0 \ (i = 1, \dots, n), & (4.30) \\ & X_{i,i} + X_{j,j} + 2X_{i,j} \ge 0 \ (1 \le i < j \le n), & (4.31) \\ & X_{i,i} + X_{j,j} - 2X_{i,j} \ge 0 \ (1 \le i < j \le n)\}. & (4.32) \end{aligned}$$

Let $\bar{X}$ be an extreme point of $\mathcal{DDT}_n^*$ and let $N(X)$ be the number of linearly independent inequalities in (4.30), (4.31) and (4.32) that are active (i.e., the equalities hold) at $X \in \mathcal{DDT}_n^*$. By the characterization of extreme points of a polyhedron (see Lemma 2.1.4), we know that

$$N(\bar{X}) = \frac{n(n+1)}{2} - 1. \tag{4.33}$$

We prove that $\bar{X}$ satisfies (4.27) by observing the active inequalities at $\bar{X}$.

It follows from $\mathrm{Tr}(\bar{X}) = 1$ that $\bar{X}$ has at least one non-zero diagonal element. This implies that the number of active inequalities in (4.30) at $\bar{X}$ is at most $n-1$. Suppose that $n-k$ inequalities in (4.30) are active at $\bar{X}$, where k is an integer and $1 \le k \le n$. Below, we show that $k \ne n$ by contradiction.

Assume that $k = n$. Then we have $\bar{X}_{i,i} > 0$ for each $1 \le i \le n$. At most one of (4.28) and (4.29) can be active at $\bar{X}$ for each $1 \le i < j \le n$. In fact, suppose that (4.28) and

(4.29) are active simultaneously for some $1 \le i < j \le n$:

$$\bar{X}_{i,i} + \bar{X}_{j,j} + 2\bar{X}_{i,j} = 0,\ \bar{X}_{i,i} + \bar{X}_{j,j} - 2\bar{X}_{i,j} = 0.$$

Then $\bar{X}_{i,j} = \bar{X}_{i,i} + \bar{X}_{j,j} = 0$ and since $\bar{X}_{i,i}, \bar{X}_{j,j} \ge 0$, we obtain $\bar{X}_{i,i} = \bar{X}_{j,j} = 0$, which is a contradiction to the assumption $\bar{X}_{i,i}, \bar{X}_{j,j} > 0$. This implies that $N(\bar{X})$ is at most $\frac{n(n-1)}{2}$, that is strictly less than the number $\frac{n(n+1)}{2} - 1$ in (4.33). This contradiction implies that $k \neq n$.

Since we have shown that $1 \le k \le n-1$, there exists a permutation matrix $P \in \mathbb{R}^{n \times n}$ such that the matrix $X^* := P\bar{X}P^T$ satisfies

$$\begin{aligned} X^*_{i,i} &= 0 \quad (1 \le i \le n-k), \\ X^*_{i,i} &> 0 \quad (n-k+1 \le i \le n). \end{aligned} \tag{4.34}$$

Note that $X^* \in \mathcal{DDT}^*_n$ and $N(X^*) = \frac{n(n+1)}{2} - 1$. Below, we show that X^* satisfies (4.27) by observing the active inequalities at X^* instead of $\bar{X}$.

Next, we show that $k = 1$; i.e., exactly $n-1$ inequalities in (4.30) are active at X^*. It follows from (4.31), (4.32) and (4.34) that $X^*_{i,j} = 0$ for each $1 \le i < j \le n-k$. This implies that all inequalities (4.28) and (4.29) with $1 \le i < j \le n-k$ at X^* are active. For each pair of (i,j) where $X_{j,j} > 0$ and $1 \le i < j$, one can show again by contradiction that at most one of (4.28) and (4.29) can be active at X^*. Consider the case when the number of active inequalities at X^* attains its maximum; i.e., exactly one of (4.28) and (4.29) is active at X^* for each pair of (i,j) where $n-k+1 \le j \le n$ and $1 \le i < j$. The following system,

$$\begin{cases} 0 = X^*_{i,i} \quad (1 \le i \le n-k), \\ 0 = X^*_{i,i} + X^*_{j,j} + 2X^*_{i,j} \quad (1 \le i < j \le n-k), \\ 0 = X^*_{i,i} + X^*_{j,j} - 2X^*_{i,j} \quad (1 \le i < j \le n-k), \\ \text{either (4.28) or (4.29) is active at } X^* \quad (n-k+1 \le j \le n,\ 1 \le i < j) \end{cases}$$

includes exactly $(n-k) + \frac{n(n-1)}{2} = \frac{n(n+1)}{2} - k$ linearly independent active inequalities. This implies that $N(X^*) \le \frac{n(n+1)}{2} - k$. By (4.33), we know that $k = 1$ and the number $\frac{n(n+1)}{2} - 1$ in (4.33) is attained only if the number of active inequalities in (4.31) and (4.32) attains its maximum.

The fact $k = 1$ implies that $X^*_{n,n} = 1$ and $X^*_{i,i} = 0$ for each $1 \le i \le n-1$; and hence $X^*_{i,j} = 0$ for each $1 \le i < j \le n-1$. Since the number of active inequalities in (4.31) and (4.32) attains its maximum, we know that either (4.28) or (4.29) is active at X^* for each (i,j) satisfying $j = n$ and $1 \le i < j$, which implies that $X^*_{i,n} \in \{\frac{1}{2}, -\frac{1}{2}\}$ for each $1 \le i < n$.

Finally, by applying the permutation $\bar{X} = P^T X^* P$, we know that there exists an integer q satisfying $1 \leq q \leq n$ for which $\bar{X}$ satisfies (4.27).

□

Lemma 4.3.10. For $n \geq 2$, let X be an extreme point of $\mathcal{DDT}_n^*$. There exist scalars $\alpha_1, \ldots, \alpha_{n-1} \in \{\frac{1}{2}, -\frac{1}{2}\}$ such that the following matrix,

$$X^* := \begin{pmatrix} 0 & & & a_1 \\ & \ddots & & \vdots \\ & & 0 & a_{n-1} \\ a_1 & \ldots & a_{n-1} & 1 \end{pmatrix} \tag{4.35}$$

satisfies

$$\|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F = \|X^* - \mathrm{P}_{\mathcal{S}_+^n}(X^*)\|_F = \frac{\sqrt{n}-1}{2}.$$

Proof. Let X be an extreme point of $\mathcal{DDT}_n^*$. By Proposition 4.3.9, there exists an integer q such that $1 \leq q \leq n$ for which X satisfies (4.27). Note that X only has one nonzero diagonal element $X_{q,q} = 1$. Let $P \in \mathbb{R}^{n \times n}$ be a permutation matrix such that $(PXP^T)_{n,n} = 1$. It is easy to see that there exist scalars $\alpha_1, \ldots, \alpha_{n-1} \in \{\frac{1}{2}, -\frac{1}{2}\}$ such that the matrix X^* defined in (4.35) satisfies $X^* = PXP^T$. Since the permutation matrix P is orthogonal, Lemma 2.1.7 implies that $Y \in \mathcal{S}_+^n$ if and only if $PYP^T \in \mathcal{S}_+^n$ for any $Y \in \mathbb{S}^n$. This fact ensures that

$$\begin{aligned} \|X - \mathrm{P}_{\mathcal{S}_+^n}(X)\|_F &= \inf_{Y \in \mathcal{S}_+^n} \|X - Y\|_F \\ &= \inf_{Y \in \mathcal{S}_+^n} \|PXP^T - PYP^T\|_F \\ &= \inf_{PYP^T \in \mathcal{S}_+^n} \|X^* - PYP^T\|_F \\ &= \|X^* - \mathrm{P}_{\mathcal{S}_+^n}(X^*)\|_F. \end{aligned} \tag{4.36}$$

By solving the eigenvalue equation $0 = |\lambda I - X^*|$ with respect to the scalar λ, we obtain that:

1. If $n = 2$, the eigenvalues of X^* are $\frac{1+\sqrt{n}}{2}$ with multiplicity 1 and $\frac{1-\sqrt{n}}{2}$ with multiplicity 1.

2. If $n \geq 3$, the eigenvalues of X^* are $\frac{1+\sqrt{n}}{2}$ with multiplicity 1, $\frac{1-\sqrt{n}}{2}$ with multiplicity 1 and 0 with multiplicity $n-2$.

From these observations, for every $n \geq 2$, X^* has only one negative eigenvalue $\lambda_{\min} := \frac{1-\sqrt{n}}{2}$;

hence,

$$\|X^* - \mathrm{P}_{\mathcal{S}^n_+}(X^*)\|_F = \sqrt{\lambda_{\min}^2} = \frac{\sqrt{n}-1}{2}. \tag{4.37}$$

We can conclude from (4.36) and (4.37) that

$$\|X - \mathrm{P}_{\mathcal{S}^n_+}(X)\|_F = \|X^* - \mathrm{P}_{\mathcal{S}^n_+}(X^*)\|_F = \frac{\sqrt{n}-1}{2}.$$

□

4.4 Evaluating approximations of the semidefinite cone by using $\mathcal{DD}^*_n$ as a reference

In the previous section, we evaluated approximations $\mathcal{DD}^*_n$ and $\mathcal{SDD}^*_n$ with the trace normalized distance (4.16), where $\mathcal{S}^n_+$ is used as a reference. Note that we find it a challenging issue to analyze the structures of all extreme points of $\mathcal{SDB}^*_n(\mathcal{H})$ for any fixed set of parameters $\{\pm 1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$. Thus, obtaining the analytical solution of $\overline{\mathrm{dist}}_T(\mathcal{SDB}^*_n(\mathcal{H}), \mathcal{S}^n_+)$ for $\{\pm 1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$ using the same idea as in Theorem 4.3.6 remains to be a challenging issue.

In this section, we evaluate approximations $\mathcal{SDD}^*_n$ and $\mathcal{SDB}^*_n(\mathcal{H})$ for some different $\mathcal{H}$ by using $\mathcal{DD}^*_n$ as a reference. Let $\mathcal{DDT}^*_n := \mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid \mathrm{Tr}(X) = 1\}$ be defined as in (4.26), and let $\mathcal{E}(\mathcal{DDT}^*_n)$ be the set of the extreme points of $\mathcal{DDT}^*_n$. We define the minimum extreme point distance from $\mathcal{DD}^*_n$ to a set $\mathcal{S}:\ \mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$ as

$$\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S}) := \inf_{X \in \mathcal{E}(\mathcal{DDT}^*_n)} \|X - \mathrm{P}_{\mathcal{S}}(X)\|_F, \tag{4.38}$$

where $\mathrm{P}_{\mathcal{S}}(X) := \mathrm{argmin}_{Y \in \mathcal{S}} \|X - Y\|_F$ is the metric projection of X on $\mathcal{S}$.

For any approximation $\mathcal{S}$ where $\mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$, the measure $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S})$ shows the minimum distance from any extreme point of $\mathcal{DDT}^*_n$ to the set $\mathcal{S}$. One can observe that for any two sets $\mathcal{S}_1, \mathcal{S}_2$ where $\mathcal{S}^n_+ \subseteq \mathcal{S}_1 \subseteq \mathcal{S}_2 \subseteq \mathcal{DD}^*_n$, we have

$$\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S}^n_+) \geq \underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S}_1) \geq \underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S}_2) \geq 0.$$

We already know from Corollary 4.3.8 that $\overline{\mathrm{dist}}_T(\mathcal{DD}^*_n, \mathcal{S}^n_+)$ attains its maximum at some point in $\mathcal{E}(\mathcal{DDT}^*_n)$. Thus the measure $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S})$ implies how far $\mathcal{S}$ is away from the farthest point from $\mathcal{DDT}^*_n$ to $\mathcal{S}^n_+$.

In what follows, we calculate $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDD}^*_n)$ and $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDB}^*_n(\mathcal{H}))$ for several different $\mathcal{H}$, including the one calculated in Section 3.2.3 and random generated others. Specifically, we firstly describe how to calculate these values for a given n, and then show the numerical results.

We know from (4.38) that for any set $\mathcal{S} : \mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$, we have

$$\underline{\text{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S}) = \inf_{\substack{X \in \mathcal{E}(\mathcal{DDT}^*_n) \\ Y \in \mathcal{S}}} \|X - Y\|_F.$$

Define a matrix

$$\bar{X} := \begin{pmatrix} 0 & & & \frac{1}{2} \\ & \ddots & & \vdots \\ & & 0 & \frac{1}{2} \\ \frac{1}{2} & \dots & \frac{1}{2} & 1 \end{pmatrix}. \tag{4.39}$$

We will use this matrix to show how to calculate the minimum extreme point distances. Similar to Lemma 4.3.10, we can prove the following lemma:

Lemma 4.4.1. Let $n \geq 2$, $\bar{X}$ be the matrix defined in (4.39), and $\mathcal{H}$ be a set of parameters where $\{\pm 1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$. Suppose that

(1) $0 \notin \mathcal{H}$,

(2) $\alpha \in \mathcal{H}$ if and only if $-\alpha \in \mathcal{H}$,

(3) $\alpha \in \mathcal{H}$ if and only if $\frac{1}{\alpha} \in \mathcal{H}$.

Then for any extreme point X of $\mathcal{DDT}^*_n$, i.e., $X \in \mathcal{E}(\mathcal{DDT}^*_n)$, we have

$$\inf_{Y \in \mathcal{SDB}^*_n(\mathcal{H})} \|X - Y\|_F = \inf_{Y \in \mathcal{SDB}^*_n(\mathcal{H})} \|\bar{X} - Y\|_F.$$

Proof. Let $I = (e_1, \dots, e_n) \in \mathbb{S}^n$ be the identity matrix. For any extreme point X of $\mathcal{DDT}^*_n$, by Proposition 4.3.9, we know that there exists an integer q satisfying $1 \leq q \leq n$ such that

$$X_{i,j} = \begin{cases} 1 & (\text{ if } i = j = q), \\ \frac{1}{2} \text{ or } -\frac{1}{2} & (\text{ if either } i = q \text{ or } j = q), \\ 0 & (\text{ otherwise}). \end{cases}$$

Similar to the proof of Lemma 4.3.10, let

$$\begin{pmatrix} 1 & 2 & \dots & n \\ \pi(1) & \pi(2) & \dots & \pi(n) \end{pmatrix}$$

be a permutation of $\{1,\dots,n\}$ with permutation matrix $P_\pi := \left(e_{\pi(1)},\dots,e_{\pi(n)}\right)^T$ such that $(P_\pi X P_\pi^T)_{n,n} = 1$. Then there exist scalars $\alpha_1,\dots,\alpha_{n-1} \in \{\frac{1}{2}, -\frac{1}{2}\}$ such that the matrix X^* defined in (4.35) satisfies $X^* = P_\pi X P_\pi^T$:

$$X^* := \begin{pmatrix} 0 & & & a_1 \\ & \ddots & & \vdots \\ & & 0 & a_{n-1} \\ a_1 & \dots & a_{n-1} & 1 \end{pmatrix} = P_\pi X P_\pi^T.$$

Since P_π is orthogonal, we have

$$\begin{aligned} \inf_{Y \in \mathcal{SDB}_n^*(\mathcal{H})} \|X - Y\|_F &= \inf_{Y \in \mathcal{SDB}_n^*(\mathcal{H})} \|P_\pi X P_\pi^T - P_\pi Y P_\pi^T\|_F \\ &= \inf_{Y \in \mathcal{SDB}_n^*(\mathcal{H})} \|X^* - P_\pi Y P_\pi^T\|_F \end{aligned} \tag{4.40}$$

Next we show that

$$Y \in \mathcal{SDB}_n^*(\mathcal{H}) \Leftrightarrow P_\pi Y P_\pi^T \in \mathcal{SDB}_n^*(\mathcal{H}). \tag{4.41}$$

We only prove the if part because the only if part can be proved similarly. For any $Y \in \mathcal{SDB}_n^*(\mathcal{H})$, by the definition (4.4), we see that for any $1 \le i \le j \le n$ and $\alpha \in \mathcal{H}$, Y satisfies

$$\langle Y, (e_i + \alpha e_j)(e_i + \alpha e_j)^T \rangle \ge 0.$$

For any $1 \le i \le j \le n$ and $\alpha \in \mathcal{H}$, we see that

$$\begin{aligned} &\langle P_\pi Y P_\pi^T, (e_i + \alpha e_j)(e_i + \alpha e_j)^T \rangle \\ =&\langle Y, P_\pi^T (e_i + \alpha e_j)(e_i + \alpha e_j)^T P_\pi \rangle \\ =&\langle Y, (e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})^T \rangle. \end{aligned} \tag{4.42}$$

If $\pi_{(i)} \le \pi_{(j)}$, one can easily observe that $(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})^T \in \mathcal{SDB}_n(\mathcal{H})$. If $\pi_{(i)} > \pi_{(j)}$, since Assumption 3 ensures that $\alpha \in \mathcal{H}$ if and only if $\frac{1}{\alpha} \in \mathcal{H}$, we have

$$(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})^T = \alpha^2 (e_{\pi_{(j)}} + \frac{1}{\alpha} e_{\pi_{(i)}})(e_{\pi_{(j)}} + \frac{1}{\alpha} e_{\pi_{(i)}})^T \in \mathcal{SDB}_n(\mathcal{H}).$$

Therefore, $(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})^T \in \mathcal{SDB}_n(\mathcal{H})$ holds. Since $Y \in \mathcal{SDB}_n^*(\mathcal{H})$, we know that

$$\langle Y, (e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})(e_{\pi_{(i)}} + \alpha e_{\pi_{(j)}})^T \rangle \ge 0.$$

Then by (4.42), we have $P_\pi Y P_\pi^T \in \mathcal{SDB}_n^*(\mathcal{H})$.

Now that (4.41) is proved, with (4.40), we have

$$\begin{aligned}\inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|X-Y\|_F &= \inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|X^*-P_\pi Y P_\pi^T\|_F \\ &= \inf_{P_\pi Y P_\pi^T\in\mathcal{SDB}_n^*(\mathcal{H})}\|X^*-P_\pi Y P_\pi^T\|_F \ (\because (4.41)) \\ &= \inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|X^*-Y\|_F \qquad (4.43)\end{aligned}$$

Furthermore, we know that there exists a diagonal matrix $Q \in \mathbb{S}^n$ where

$$Q_{i,i} = \begin{cases} -1 & (\text{ if } a_i = -\frac{1}{2}), \\ 1 & (\text{ otherwise}), \end{cases}$$

such that $QX^*Q^T = \bar{X}$. It is obvious that Q is orthogonal, and one can show without too much effort that

$$Y \in \mathcal{SDB}_n^*(\mathcal{H}) \Leftrightarrow QYQ^T \in \mathcal{SDB}_n^*(\mathcal{H}). \qquad (4.44)$$

Then we have

$$\begin{aligned}\inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|X^*-Y\|_F &= \inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|\bar{X}-QYQ^T\|_F \\ &= \inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|\bar{X}-Y\|_F. \ (\because (4.41)) \qquad (4.45)\end{aligned}$$

With (4.43) and (4.45), we can conclude that for any extreme point X of $\mathcal{DDT}_n^*$,

$$\inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|X-Y\|_F = \inf_{Y\in\mathcal{SDB}_n^*(\mathcal{H})}\|\bar{X}-Y\|_F.$$

□

Similar to Lemma 4.4.1, we can prove Lemma 4.4.2. In fact, the only difference between the proof of Lemma 4.4.1 and Lemma 4.4.2 is that, instead of using (4.41) and (4.44), we need the facts $Y \in \mathcal{SDD}_n^* \Leftrightarrow P_\pi Y P_\pi^T \in \mathcal{SDD}_n^*$ and $Y \in \mathcal{SDD}_n^* \Leftrightarrow QYQ^T \in \mathcal{SDD}_n^*$ to show Lemma 4.4.2, which are not hard to see.

Lemma 4.4.2. Let $n \geq 2$, $\bar{X}$ be the matrix defined in (4.39). Then for any extreme point X of $\mathcal{DDT}_n^*$, i.e., $X \in \mathcal{E}(\mathcal{DDT}_n^*)$, we have

$$\inf_{Y\in\mathcal{SDD}_n^*}\|X-Y\|_F = \inf_{Y\in\mathcal{SDD}_n^*}\|\bar{X}-Y\|_F.$$

Let $\mathcal{H}$ be a set of parameters satisfying Assumptions (1-3) in Lemma 4.4.1. Lemma 4.4.1 and Lemma 4.4.2 shows that

$$\begin{aligned}\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H})) &= \inf_{Y \in \mathcal{SDB}_n^*(\mathcal{H})} \|\bar{X} - Y\|_F, \\ \underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*) &= \inf_{Y \in \mathcal{SDD}_n^*} \|\bar{X} - Y\|_F.\end{aligned}$$

This gives us a way to numerically calculate $\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H}))$ and $\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*)$ by solving the following second order cone programs (SOCP) for any given $n \geq 2$:

$$\begin{aligned}\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H})) = \min\ & \|\bar{X} - Y\|_F \\ \text{s.t. } & Y_{i,i} + \alpha^2 Y_{j,j} + 2\alpha Y_{i,j} \geq 0 \ (1 \leq i \leq j \leq n,\ \alpha \in \mathcal{H}), \\ & Y \in \mathbb{S}^n. \\ \underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*) = \min\ & \|\bar{X} - Y\|_F \\ \text{s.t. } & \begin{pmatrix} Y_{i,i} & Y_{i,j} \\ Y_{i,j} & Y_{j,j} \end{pmatrix} \in \mathcal{S}_+^2 \ (1 \leq i < j \leq n), \\ & Y \in \mathbb{S}^n.\end{aligned}$$

Note that Definition (4.4) gives the characterization of $\mathcal{SDB}_n^*(\mathcal{H})$, and we refer to Corollary 3.1.20 and Lemma 3.1.9 for the characterization of $\mathcal{SDD}_n^*$ in the SOCP formulations above.

In our numerical experiment, the above SOCPs are solved by using the Gurobi Optimizer 9.0.0 [53]. The following table shows the numerical result of the minimum extreme point distances from $\mathcal{DD}_n^*$ to $\mathcal{S}_+^n$, $\mathcal{SDD}_n^*$, and $\mathcal{SDB}_n^*(\mathcal{H})$ with different $\mathcal{H}$, including the one calculated in Section 3.2.3 and random generated others:

$$\begin{aligned}\bar{\mathcal{H}} =& \{\pm 1, \pm 1 \pm \sqrt{2}\}, \\ \mathcal{H}_1 =& \{\pm 1, \pm 10, \pm 0.1\}, \\ \mathcal{H}_2 =& \{\pm 1, \pm 1.25, \pm 0.8\}.\end{aligned}$$

Note that these sets of parameters satisfy Assumptions (1)-(3) in Lemma 4.4.1. Also, we would like to notice that Proposition 4.3.9 and Lemma 4.3.10 ensures that

$$\begin{aligned}\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n) =& \overline{\mathrm{dist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n), \\ =& \frac{\sqrt{n} - 1}{2}.\end{aligned}$$

Thus $\underline{\mathrm{Edist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$ in Table 4.4 is calculated directly as above.

Table 4.1: The minimum extreme point distance from $\mathcal{DD}_n^*$ to $\mathcal{S}_+^n$ and other sets for $n = 2\ldots,50$.

n	2	10	20	30	40	50
$\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$	0.207	1.081	1.736	2.239	2.662	3.036
$\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*)$	0.207	0.582	0.803	0.954	1.072	1.171
$\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\bar{\mathcal{H}}))$	0.207	0.574	0.767	0.882	0.960	1.018
$\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H}_1))$	0.089	0.267	0.388	0.479	0.555	0.622
$\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H}_2))$	0.098	0.197	0.220	0.229	0.234	0.237

We also give a figure that illustrates the minimum extreme point distances from $\mathcal{DD}_n^*$ to $\mathcal{S}_+^n$ and other sets for different n.

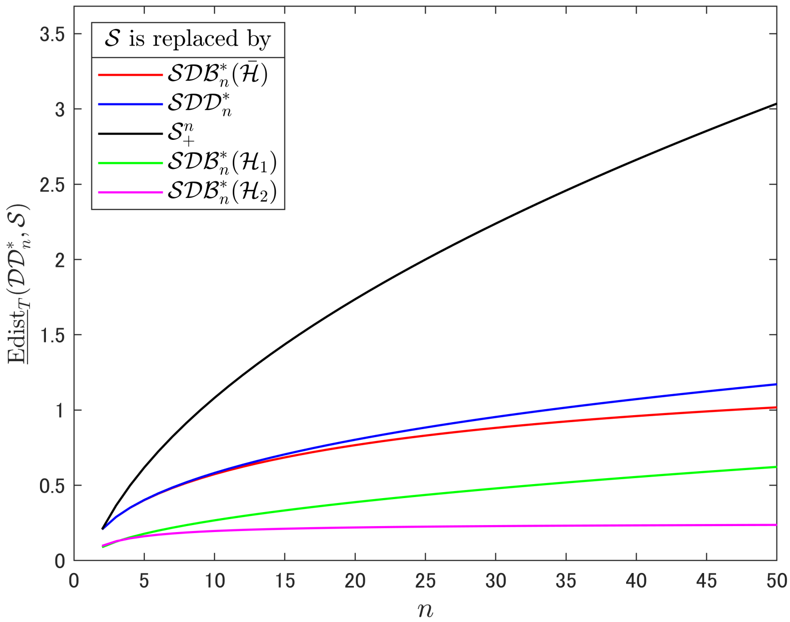


Figure 4.2: The minimum extreme point distance from $\mathcal{DD}_n^*$ to $\mathcal{S}_+^n$, $\mathcal{SDD}_n^*$ and $\mathcal{SDB}_n^*(\bar{\mathcal{H}})$ with different $\mathcal{H}$ for $n = 2, \ldots, 50$.

As can be seen in Table 4.4 and Figure 4.2, when $n = 2$, $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{S}_+^n)$, $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*)$ and $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\bar{\mathcal{H}}))$ are the same, while $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H}_1))$ and $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\mathcal{H}_2))$ are closer to 0. When n becomes larger, we can observe that $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDB}_n^*(\bar{\mathcal{H}}))$ is smaller than $\underline{\text{Edist}}_T(\mathcal{DD}_n^*, \mathcal{SDD}_n^*)$ but stays very close to the latter for each n. For all $n = 2, \ldots, 50$, $\mathcal{SDB}_n^*(\mathcal{H}_1)$ and $\mathcal{SDB}_n^*(\mathcal{H}_2)$ are the closest to the extreme points of $\mathcal{DD}_n^*$.

4.5 Conclusion

In this Chapter, we first showed that the norm normalized distance $\overline{\mathrm{dist}}_F(\mathcal{S}, \mathcal{S}^n_+)$ has the same value whenever $\mathcal{SDD}^*_n \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$, since $\overline{\mathrm{dist}}_F(\mathcal{DD}^*_n, \mathcal{S}^n_+) = \overline{\mathrm{dist}}_F(\mathcal{SDD}^*_n, \mathcal{S}^n_+)$ holds. This implies that the norm normalized distance is not a sufficient measure to evaluate these approximations. As a new measure to compensate for the weakness of that distance, we proposed a new distance, the trace normalized distance $\overline{\mathrm{dist}}_T(\mathcal{S}, \mathcal{S}^n_+)$. Using this new measure, we proved that $\overline{\mathrm{dist}}_T(\mathcal{DD}^*_n, \mathcal{S}^n_+)$ and $\overline{\mathrm{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+)$ are different, i.e., $\overline{\mathrm{dist}}_T(\mathcal{DD}^*_n, \mathcal{S}^n_+) = \frac{\sqrt{n}-1}{2}$ and $\overline{\mathrm{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+) = \frac{n-2}{n}$.

Table 4.2 compares the proof techniques used by Blekherman et al. [20] and those in Sections 4.2 and 4.3 of this chapter.

Table 4.2: Comparison of proof techniques in [20] and those in this chapter.

Proof techniques of each theorem		Blekherman et al. 2020 [20]
Object		$\mathcal{S}^{n,k}$
$\overline{\mathrm{dist}}_F(\cdot, \mathcal{S}^n_+)$	Upper bound	(Theorem 1) Averaging technique
		(Theorem 2) Bound the most negative eigenvalue
	Lower bound	(Theorem 3) Construct a matrix far from $\mathcal{S}^n_+$
		(Theorem 4) Restricted Isometry Property

Proof techniques of each theorem		This paper	
Object		$\mathcal{SDD}^*_n$	$\mathcal{DD}^*_n$
$\overline{\mathrm{dist}}_F(\cdot, \mathcal{S}^n_+)$	Upper bound	(Theorem 4.2.1) $\overline{\mathrm{dist}}_F(\mathcal{SDD}^*_n, \mathcal{S}^n_+) \leq \overline{\mathrm{dist}}_F(\mathcal{DD}^*_n, \mathcal{S}^n_+)$	(Theorem 4.2.1) Averaging technique
	Lower bound	(Theorem 4.2.1) Corollary of Theorem 3 [20]	(Theorem 4.2.1) $\overline{\mathrm{dist}}_F(\mathcal{DD}^*_n, \mathcal{S}^n_+) \geq \overline{\mathrm{dist}}_F(\mathcal{SDD}^*_n, \mathcal{S}^n_+)$
$\overline{\mathrm{dist}}_T(\cdot, \mathcal{S}^n_+)$	Upper bound	(Lemma 4.3.5) Averaging technique	(Theorem 4.3.6) Analyze extreme points of $\mathcal{DDT}^*_n$ and use the Bauer maximum principle
	Lower bound	(Lemma 4.3.4) Construct a matrix far from $\mathcal{S}^n_+$	

Then, we proposed a new measure that evaluate an approximation $\mathcal{S}$: $\mathcal{S}^n_+ \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$ by calculating the minimum distance from any extreme point of $\mathcal{DDT}^*_n$ to the set $\mathcal{S}$, namely $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S})$. We described how to calculate $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \cdot)$ for approximations $\mathcal{SDB}^*_n(\mathcal{H})$ and $\mathcal{SDD}^*_n$ for any given $n \geq 2$. One can observe from the numerical results that $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDB}^*_n(\bar{\mathcal{H}}))$ stays very close to $\underline{\mathrm{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDD}^*_n)$ for each n.

Chapter 5

Cutting-plane methods for solving semidefinite optimization problems

In this chapter, we first introduce the cutting-plane method for solving SDPs, referring to Ahmadi et al. [1], and focus on the approximations of the semidefinite cone in this method. Then we conduct numerical experiments to show the result of the cutting-plane methods using different initial relaxations on random Doubly Non-Negative (DNN) problems and Maximum stable set problem. The contents in Section 5.2.2 are based on the recent paper [114].

5.1 A cutting-plane plane method for solving SDPs

We consider the standard SDP of the form:

$$\begin{aligned} \min\ & \langle C, X\rangle \\ \text{s.t. } & \langle A_j, X\rangle = b_j, j = 1, 2, \ldots, m, \\ & X \in \mathcal{S}^n_+, \end{aligned} \tag{5.1}$$

where $C, A_j \in \mathbb{S}^n$, $b_j \in \mathbb{R}$ $(j = 1, \ldots, m)$.

To introduce the cutting-plane method for solving (5.1), we assume that

Assumption 5.1.1. All feasible solution X to Problem (5.1) satisfies $\mathrm{Tr}(X) \le T$ for some positive scalar T.

If the feasible region of Problem (5.1) is empty, then the problem is infeasible. Otherwise, Assumption 5.1.1 ensures that the feasible region of Problem (5.1) is nonempty and compact (i.e., bounded and closed). Then Weierstrass's Theorem (e.g., Prop.A.2.7 [15]) implies that Problem (5.1) has a bounded optimal value. Note that Assumption 5.1.1 is often naturally satisfied, e.g., the SDP relaxations of the maximum stable set problem and the max-cut problem. Also, one may notice that this assumption can be approximately satisfied by adding a big-M constraint $\mathrm{Tr}(X) \leq M$ in Problem (5.1) for a large positive scalar M.

We briefly introduce the cutting-plane method by Ahmadi et al. [1] on the SDP (5.1). Let $\mathcal{P}^n$ be an outer approximation of $\mathcal{S}^n_+$, i.e., $\mathcal{S}^n_+ \subseteq \mathcal{P}^n \subseteq \mathbb{S}^n$, and replace $X \in \mathcal{S}^n_+$ by $X \in \mathcal{P}^n$ in (5.1). Then, we obtain a relaxation of (5.1):

$$\begin{aligned} \min\ & \langle C, X \rangle \\ \text{s.t.}\ & \langle A_j, X \rangle = b_j, j = 1, 2, \ldots, m, \\ & X \in \mathcal{P}^n, \end{aligned} \tag{5.2}$$

The relaxed problem (5.2) is expected to be easier to solve and to give us a finite lower bound of problem (5.1). Specifically, we assume that $\mathcal{P}^n$ is chosen such that

Assumption 5.1.2. The feasible region of the relaxed problem (5.2) is bounded under Assumption 5.1.1.

By solving the initial relaxed problem (5.2), we can obtain its optimal solution X^*. To get a better lower bound, we select some eigenvectors with negative eigenvalues of X^*, say $d_1, .., d_k$. By adding cutting-planes

$$\langle d_i d_i^T, X \rangle \geq 0 \quad (i = 1, .., k)$$

to problem (5.2), we can obtain a new optimization problem

$$\begin{aligned} \min\ & \langle C, X \rangle \\ \text{s.t.}\ & \langle A_j, X \rangle = b_j,\ j = 1, 2, \ldots, m, \\ & \langle d_i d_i^T, X \rangle \geq 0,\ i = 1, .., k, \\ & X \in \mathcal{P}^n. \end{aligned} \tag{5.3}$$

Notice that the optimal solution X^* of problem (5.2) is cut from the feasible region of problem (5.3) since $\langle d_i d_i^T, X^* \rangle < 0$ $(i = 1, .., k)$. On the other hand, since

$$\begin{aligned} \mathcal{S}^n_+ &= \{X \in \mathbb{S}^n \mid \forall d \in \mathbb{R}^n,\ \langle dd^T, X \rangle \geq 0\} \\ &\subseteq \mathcal{P}^n \cap \{X \in \mathbb{S}^n \mid \langle d_i d_i^T, X \rangle \geq 0\ (i = 1, .., k)\}, \end{aligned}$$

every feasible solution of (5.1) is feasible for (5.3), and hence problem (5.3) is a relaxation of problem (5.1). These facts ensure that problem (5.3) is a tighter relaxation of problem

(5.1) than problem (5.2). By repeating this procedure, we are able to obtain a series of non-decreasing lower bounds of (5.1). If we obtain an optimal solution of Problem (5.3), denoted as $\bar{X}$, whose smallest eigenvalue: $\lambda_{\min}(\bar{X})$ satisfies $\lambda_{\min}(\bar{X}) > -\epsilon$ for a given tolerance $\epsilon > 0$, then we call $\bar{X}$ an ϵ-optimal solution of Problem (5.1). Note that since the eigenvectors are usually dense, we only have to add eigenvectors corresponding to up to the second smallest eigenvalues to $\{d_i\}$ at every iteration, which increases computational efficiency. The above mentioned cutting-plane method for solving Problem (5.1) is summarized in Algorithm 1.

Algorithm 1 Cutting-plane method for solving SDPs

Step 0 (Initialization) Let $\epsilon > 0$ be a tolerance for feasibility, and let $\mathcal{P}_0^n$ be an initial outer approximation of $\mathcal{S}_+^n$ satisfying Assumption 5.1.2. Set $k \leftarrow 0$

Step 1 (Optimization) Solve the relaxed problem:

$$\begin{aligned} \min\ & \langle C, X\rangle \\ \text{s.t. } & \langle A_j, X\rangle = b_j, j = 1, 2, \ldots, m, \\ & X \in \mathcal{P}_k^n, \end{aligned} \tag{5.4}$$

and obtain its optimal solution X_k^*.

Step 2 (Termination check)

(1) If the relaxed problem (5.4) is infeasible, then Problem (5.1) is infeasible.

(2) If the smallest eigenvalue of X_k^*: $\lambda_{\min}(X_k^*)$ satisfies $\lambda_{\min}(X_k^*) > -\epsilon$, then X_k^* is an ϵ-optimal solution of Problem (5.1).

Step 3 (Cut generation) Let d_k^1 and d_k^2 be the eigenvectors corresponding to up to the second smallest eigenvalues of X_k^*. Set

$$\mathcal{P}_{k+1}^n \leftarrow \mathcal{P}_k^n \cap \{X \in \mathbb{S}^n \mid \langle d_k^1(d_k^1)^T, X\rangle \geq 0,\ \langle d_k^2(d_k^2)^T, X\rangle \geq 0\}.$$

Step 4 Set $k \leftarrow k + 1$ and return to Step 1.

Since the work of Kelly [65], several authors have given the proof of convergence of general cutting-plane methods [14, 17, 81, 89]. We refer to Theorem 1 of Bertsimas and Cory-Wright [17] for a proof of convergence of Algorithm 1 with $\mathcal{SDD}_n^*$ as its initial approximation. The convergence of Algorithm 1 with $\mathcal{DD}_n^*$ or $\mathcal{SDB}_n^*$ as its initial approximation can be proved similarly. Based on Theorem 1 of Bertsimas and Cory-Wright [17], we give a proof of convergence of Algorithm 1 here for completeness.

Theorem 5.1.3. Suppose that (5.1) is feasible and Assumption 5.1.1 holds. Also assume that the initial approximation $\mathcal{P}_0^n$ in Algorithm 1 is chosen such that Assumption 5.1.2 holds, i.e., all feasible point X of the initial relaxed problem (5.4) is bounded by a positive scalar R: $\|X\|_F \leq R$. Then for any tolerance $\epsilon > 0$, Algorithm 1 terminates within finite iterations.

Proof. Let X_k^* be a feasible solution returned by the kth iteration of Algorithm 1 and let

d_k be the eigenvector corresponding to the smallest eigenvalues of X_k^*. Let $\epsilon > 0$ be a given tolerance. Suppose that at some iteration $k > 1$, Algorithm 1 has not converged. Then we know that for all $i < k$,

$$\lambda_{\min}(X_i^*) = \langle X_i^*, d_i d_i^T \rangle < -\epsilon.$$

Since X_k^* is a feasible solution to (5.4), we have that for all $i < k$,

$$\langle X_k^*, d_i d_i^T \rangle \geq 0.$$

Then for each $i < k$, we have

$$\begin{aligned}
\|X_k^* - X_i^*\|_F &= \|X_k^* - X_i^*\|_F \|d_i d_i^T\|_F \ (\because \|d_i\|_2 = 1) \\
&\geq |\langle X_k^* - X_i^*, d_i d_i^T \rangle| \ (\because \text{Cauchy-Schwarz inequality}) \\
&= |\langle X_k^*, d_i d_i^T \rangle - \langle X_i^*, d_i d_i^T \rangle| \\
&> \epsilon.
\end{aligned}$$

This implies that for each $i < k$, the hyperplane $\{Y \in \mathbb{S}^n \mid \langle Y, d_i d_i^T \rangle = -\frac{\epsilon}{2}\}$ strictly separates X_k^* and X_i^*. Thus for each $i < k$, the Euclidean ball of radius $\frac{\epsilon}{2}$ centered at X_i^* (i.e., $\{Y \in \mathbb{S}^n \mid \|X_i^* - Y\|_F \leq \frac{\epsilon}{2}\}$) has an empty intersection with the ball of the same radius centered at X_k^*. This also implies that any two of these balls will not overlap. The volume of a ball of radius r in $\mathbb{R}^n$ is $\frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)} r^n$, where $\Gamma(\cdot)$ is the Gamma function (e.g., [78]). Then for $i \leq k$, the combined volume of balls of radius $\frac{\epsilon}{2}$ centered at X_i^* in $\mathbb{R}^{n \times n}$ is

$$\text{Vol}_1 := k \frac{\pi^{\frac{n^2}{2}}}{\Gamma(\frac{n^2}{2} + 1)} (\frac{\epsilon}{2})^{n^2}.$$

By the assumption of this theorem, we have that every feasible point X of the initial relaxed problem (e.g., $X_1^*, \ldots, X_k^*$) is bounded by a positive scalar R: $\|X\|_F \leq R$. Then, the balls of radius $\frac{\epsilon}{2}$ centered at $X_1^*, \ldots, X_k^*$ are contained in a ball of radius $R + \frac{\epsilon}{2}$ centered at the origin, which has volume

$$\text{Vol}_2 := \frac{\pi^{\frac{n^2}{2}}}{\Gamma(\frac{n^2}{2} + 1)} (R + \frac{\epsilon}{2})^{n^2}.$$

Hence, if Algorithm 1 has not converged at iteration k, then $\text{Vol}_1 < \text{Vol}_2$ will imply that

$$k < (\frac{2R}{\epsilon} + 1)^{n^2}.$$

This shows that for any $\epsilon > 0$, Algorithm 1 will converge to an ϵ-optimal solution after $(\frac{2R}{\epsilon}+1)^{n^2}$ iterations.

□

As for the selection of the initial relaxation $\mathcal{P}^n$, we are ready to use our proposed approximation of $\mathcal{S}^n_+$ based on the expanded SD bases. Let $\bar{\mathcal{H}} := \{\pm 1, \pm 1 \pm \sqrt{2}\}$ be the set of parameters calculated in Section 3.2.3, and simply let $\mathcal{SDB}_n$ denote the conical hull of expanded SD bases using $\bar{\mathcal{H}}$:

$$\mathcal{SDB}_n := \text{cone}\left(\bigcup_{\alpha\in\bar{\mathcal{H}}} \bar{\mathcal{B}}_n(\alpha)\right).$$

Then, as has been described in the Corollary 3.2.7, we have

$$\mathcal{S}^n_+ \subseteq \mathcal{SDD}^*_n \subseteq \mathcal{SDB}^*_n \subseteq \mathcal{DD}^*_n. \tag{5.5}$$

Bertsimas and Cory-Wright [17] proved that if $\mathcal{DD}^*_n$ is selected to be the initial outer approximation $\mathcal{P}_n$ in Problem (5.2), with Assumption 5.1.1, Assumption 5.1.2 is satisfied. Since $\mathcal{SDD}^*_n$ and $\mathcal{SDB}^*_n$ are subsets of $\mathcal{DD}^*_n$, we know that if $\mathcal{SDD}^*_n$ or $\mathcal{SDB}^*_n$ is selected to be the initial outer approximation $\mathcal{P}_n$, Assumption 5.1.2 will also be satisfied. Thus, $\mathcal{DD}^*_n$, $\mathcal{SDD}^*_n$ and $\mathcal{SDB}^*_n$ are suitable candidates for the choice of $\mathcal{P}_n$.

If $\mathcal{SDB}^*_n$ or $\mathcal{DD}^*_n$ is selected to be $\mathcal{P}_n$, the corresponding relaxed problem in the cutting-plane procedure becomes an LP, which allows us to use powerful state-of-the-art LP solvers, such as Gurobi [53]. Ahmadi et al. [1] showed that when $\mathcal{SDD}^*_n$ is selected, the relaxations turn out to be SOCPs. Although $\mathcal{SDD}^*_n$ provides a tighter relaxation than either $\mathcal{DD}_n$ or $\mathcal{SDB}_n$, the latter two relaxations are expected to have a lower computational cost. In addition, in [1], Ahmadi et al. also proposed an SOCP-based cutting-plane approach, named SDSOS. Instead of adding 2 linear cuts, SDSOS adds an SOCP cut at every iteration. Specifically, they used the eigenvector corresponding to 2 smallest eigenvalues, namely $d^1, d^2 \in \mathbb{R}^n$, of a relaxed solution X^* at each iteration, and construct the following cut :

$$(d^1, d^2)^T X^* (d^1, d^2) \in \mathcal{S}^2_+.$$

This cut can be equivalently transformed into 2 linear cuts and 1 SOCP cut.

We conducted experiments to compare the efficiencies of Algorithm 1 using different approximations and SDSOS. The specifications of the experimental methods are summarized in Table 5.1.

Table 5.1: Specifications of the experimental methods

Method	$\mathcal{P}^n$	Number of cuts added at each iteration		Solver
		LP cut	SOCP cut	
CPDD	$\mathcal{DD}_n^*$	2	0	Gurobi
CPSDB	$\mathcal{SDB}_n^*$	2	0	Gurobi
CPSDD	$\mathcal{SDD}_n^*$	2	0	Mosek
SDSOS	$\mathcal{SDD}_n^*$	2	1	Mosek

5.2 Numerical experiments

5.2.1 Random instances of DNN problems

In this section, we apply Algorithm 1 with different initial approximations to random generated Doubly Non-Negative (DNN) problem of the form:

$$\begin{aligned} &\min\ \langle C, X\rangle \\ &\text{s.t. } \langle A_j, X\rangle = b_j, j = 1, 2, \ldots, m, \\ &\quad X \in \mathcal{S}_+^n \cap \mathcal{N}^n, \end{aligned} \tag{5.6}$$

where $C, A_j \in \mathbb{S}^n$, $b_j \in \mathbb{R}$ $(j = 1 \ldots, m)$ and $\mathcal{N}^n$ is the set of $n \times n$ nonnegative symmetric matrices. The dual of this problem is given by

$$\begin{aligned} &\min\ b^T y \\ &\text{s.t. } C - \sum_{j=1}^m y_j A_j = S, \\ &\quad S \in \mathcal{S}_+^n + \mathcal{N}^n. \end{aligned}$$

Following Yamashita et al. [120], we generated random instances of Problem (5.6) as follows. First, we generated $V \in \mathbb{R}^{n\times k_1}$ and $W \in \mathbb{R}^{n\times k_2}$ with random integers $1 \le k_1, k_2 \le n$, where each element of V, W was drawn from a uniform distribution in $[0.1, 1]$. Let I be the identity matrix, and let $X_0 := VV^T + 0.1I$ to be a primal interior feasible solution and $S_0 := WW^T + 0.1I$ to be a slack variable. Let $B \in \mathcal{N}^n$ be a symmetric matrix whose elements were drawn from a uniform distribution in $[0, 1]$, and let $A_1 := 0.1I + B$. Each element of the dual feasible solution $y_0 \in \mathbb{R}^m$ and $A_j \in \mathbb{S}^n$ $(j = 2, 3, \ldots, m)$ was chosen from a uniform distribution in $[-1, 1]$. Here, let $C = S_0 + \sum_{j=1}^m y_j A_j$ and $b_j = \langle A_j, X_0\rangle$ $(j = 1, 2, \ldots, m)$. Then (y_0, X_0, S_0) is a primal-dual interior feasible solution of the DNN problem (5.6). By the strong duality theorem of conic optimization problems (Theorem 2.2.1), we know that the resulting DNN problem has no duality gap. Note that for any feasible solution X of this problem, since $\langle B, X\rangle \geq 0$, we have

$$\mathrm{Tr}(X) = \langle I, X\rangle \leq \langle I, X\rangle + 10\langle B, X\rangle = 10\langle A_1, X\rangle = 10b_1.$$

This implies that the above generated instances of (5.6) satisfies Assumption 5.1.1.

We apply cutting-plane methods listed in Table 5.1 to (5.6) with $n = 100, 150, 200$ and $m = 10, 50$. The stopping criteria is set to be $\epsilon := 10^{-6}$. All experiments were performed with MATLAB 2018b on a Windows PC with an Intel(R) Core(TM) i7-6700 CPU running at 3.4 GHz and 16 GB of RAM. The LPs were solved using Gurobi Optimizer 9.0.0 [53] and the SOCPs and SDPs are solved using Mosek Optimizer 9.0 [6].

We evaluate the efficiency of each method by using the gap between the lower bounds of this method and the optimal value of (5.8). Let f^* be the optimal value of (5.6). For any method listed in Table 5.1, at iteration k, we denoted the lower bound of (5.6) as f_k. We used the value $\left|\frac{f^*-f_k}{f^*}\right| \times 100\%$ to evaluate the accuracy of each iteration and called it the *Gap*. Note that when solving SOCPs in our experiments, Mosek cannot obtain useful solution sometimes due to numerical errors. In this case, e.g., when Mosek outputs error code '10006' at iteration k, we set $f_k := f_{k-1}$. The numerical results are shown in Figure 5.1, Figure 5.2 and Table 5.2.

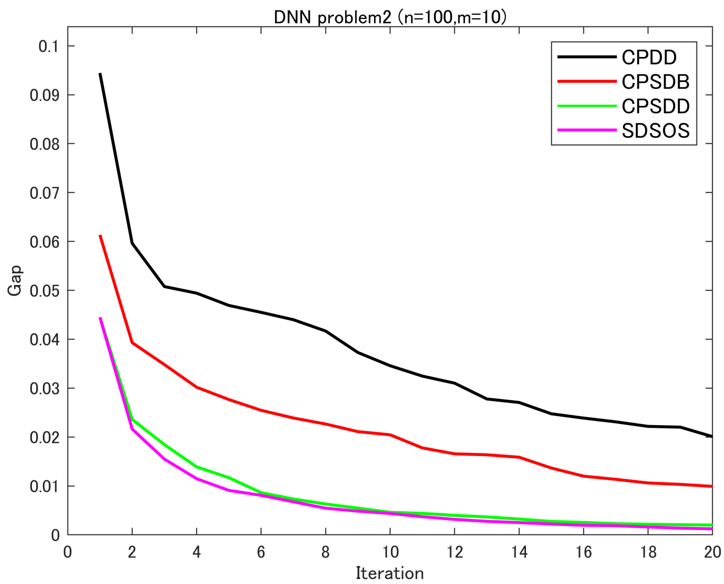


Figure 5.1: Relation between the number of iterations and the gap for a random instance of DNN problem

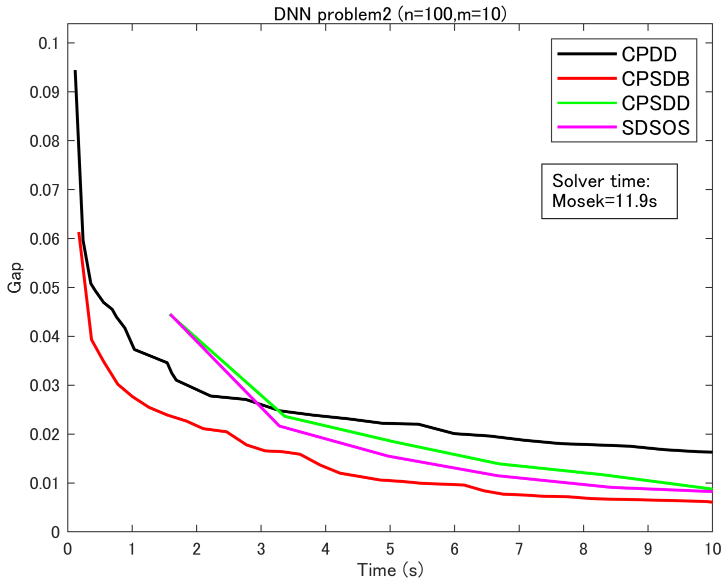


Figure 5.2: Relation between the computational time and the gap for the same random instance of DNN problem

Figure 5.1 shows the result for an instance with $n = 100$ and $m = 10$. The x-axis is the number of iterations, and the y-axis is the gap between the lower bounds of each method and the SDP bound obtained by (5.6). As can be seen in this figure, the gap obtained by CPSDB is much better than the gap generated by CPDD at each iteration. Although SDSOS adds an extra SOCP cut at every iteration and takes longer to solve, the gap obtained by SDSOS is only slightly better than CPSDD at each iteration.

Figure 5.2 shows the efficiency of each method for the same instance with $n = 100$ and $m = 10$. The x-axis is the computational time, and the y-axis is the gap. As can be seen in this figure, the most efficient method is CPSDB. CPSDB attained a lower bound with gap around 2.7% within 1 s, while CPDD attained a lower bound with gap around 4% after the same amount of time. Note that the first iteration took 1.58 s for CPSDD and SDSOS to solve and the initial gap attained is 4.45%.

Table 5.2 gives numerical results for all instances, where k is the instance number and 'Ite' represents the number of iteration. The gaps obtained at the first and fifth iterations for each method and their computational time are given. We also present the gap achieved by each method after a fixed time of computation.

As can be seen in this table, for every random instance, CPSDB has a better gap than CPDD at every iteration. Although methods using SOCPs (CPSDD, SDSOS) obtain better lower bounds than methods using LPs (CPDD, CPSDB) at every iteration, it takes them much longer than those LP methods to solve each iteration.

For all instances with $m = 50$, CPSDB achieved the best lower bounds within the same amount of time. For example, for the problem with $(n, m, k) = (150, 50, 1)$, after 60 s of computation, CPSDB obtained a lower bound whose gap is 2.93%, while CPDD, CPSDD, and SDSOS got gaps greater than 3.44%. This indicates that the method with our approximation $\mathcal{SDB}_n^*$ may be efficient for solving DNN problems with a large number of constraints. For instances with $n = 100$ and $m = 10$, CPSDB gave the best lower bounds within the same amount of time. CPDD showed the best result after a fixed time of computation for most instances with $n = 150, 200$ and $m = 10$, while CPSDB again showed its efficiency for the instance with $(n, m, k) = (150, 50, 1)$.

Mosek efficiently solved instances with $n = 100$ directly, but as shown in the table, instances with $n = 150, 200$ required a significant amount of time for Mosek to solve. One may consider using the cutting-plane method CPSDB with our polyhedral approximation $\mathcal{SDB}_n$ to obtain efficient lower bounds of large-scale SDPs in a reasonable time.

Table 5.2: Numerical results for solving random DNN problems

(n,m,k)	Mosek	ite	CPDD		CPSDB		CPSDD		SDSOS	
	Time (s)		Gap (%)	Time (s)	Gap (%)	Time (s)	Gap (%)	Time (s)	Gap (%)	Time (s)
(100,10,1)	13.26	1	4.04	0.12	2.15	0.16	0.72	1.63	0.72	1.63
		5	2.04	0.51	1.00	0.89	0.14	8.56	0.14	8.82
			0.04	10	0.01	10	0.14	10	0.14	10
(100,10,2)	12.52	1	9.44	0.12	6.13	0.17	4.45	1.58	4.45	1.59
		5	4.69	0.56	2.77	1.00	1.17	8.29	0.91	8.44
			1.64	10	0.62	10	1.17	10	0.91	10
(100,50,1)	28.05	1	14.7	0.71	11.15	0.81	9.98	2.03	9.98	2.06
		5	9.30	3.62	7.88	3.94	6.54	11.45	6.41	11.65
			6.24	20	4.74	20	5.74	20	5.48	20
(100,50,2)	34.66	1	10.12	0.65	7.48	0.77	6.69	2.11	6.69	2.13
		5	6.25	3.46	4.28	4.02	3.66	11.97	3.54	12.70
			3.87	20	2.92	20	3.17	20	3.13	20
(150,10,1)	124.98	1	6.04	0.12	4.01	0.33	3.02	4.61	3.02	4.68
		5	2.33	0.65	1.17	2.02	0.42	24.03	0.31	24.18
			3e-4	30	0.02	30	0.31	30	0.25	30
(150,10,2)	132.19	1	7.12	0.13	4.45	0.43	2.54	4.63	2.54	4.65
		5	3.35	0.73	2.07	2.44	0.87	23.67	0.70	23.76
			0.04	30	0.23	30	0.72	30	0.54	30
(150,50,1)	255.01	1	8.44	1.79	6.76	2.32	6.07	6.57	6.07	6.69
		5	6.35	8.71	4.67	11.37	4.05	35.73	4.37	24.93
			3.45	60	2.93	60	3.44	60	3.67	60
(150,50,2)	237.34	1	10.00	1.77	7.80	2.60	6.83	7.07	6.83	7.09
		5	7.40	8.76	5.63	12.83	5.88	20.48	5.12	24.89
			4.57	60	3.99	60	4.36	60	4.39	60
(200,10,1)	588.96	1	14.29	0.24	10.01	0.71	6.87	9.31	6.87	9.46
		5	8.57	1.27	4.39	4.87	2.45	49.46	2.42	50.37
			0.14	90	0.82	90	1.94	90	1.63	90
(200,10,2)	871.41	1	17.41	0.71	14.37	0.54	8.57	8.91	8.57	8.97
		5	9.24	3.63	5.18	3.04	3.16	48.06	2.66	47.14
			0.91	90	0.59	90	2.06	90	1.46	90
(200,50,1)	1176.10	1	11.71	3.24	8.87	4.38	7.38	15.48	7.38	15.48
		5	7.95	16.12	5.94	28.12	6.29	46.95	5.26	71.48
			4.56	180	4.37	180	5.66	180	5.26	180
(200,50,2)	967.41	1	17.64	4.52	14.14	4.54	11.96	15.07	11.96	15.14
		5	10.62	23.00	8.01	23.45	8.63	46.84	8.59	46.24
			5.56	180	4.80	180	6.14	180	5.37	180

5.2.2 Maximum stable set problem

Conic optimization problems, including SDPs and copositive programs, have been shown to provide tight bounds for NP-hard combinatorial and nonconvex optimization problems. Here, we consider applying approximations of $\mathcal{S}_+^n$ to one of those NP-hard problems, the maximum stable set problem. A stable set of a graph $G(V,E)$ is a set of vertices in V, such that there is no edge connecting any pair of vertices in the set. The maximum stable set problem aims to find the stability number, i.e., the number of vertices of the largest stable set of G, namely $\alpha(G)$.

De Klerk and Pasechnik [38] proposed a copositive programming formulation to obtain the exact stability number of a graph G with n vertices:

$$\begin{aligned} \alpha(G) = \max\ & \langle ee^T, X\rangle \\ \text{s.t. } & \langle A+I, X\rangle = 1, \\ & X \in \mathcal{C}_n^*, \end{aligned} \tag{5.7}$$

where $e := (1,\dots,1)^T$ and A is the adjacency matrix of graph G, and $\mathcal{C}_n^*$ is the dual cone of the copositive cone $\mathcal{C}_n := \{X \in \mathbb{S}^n \mid d^T X d \geq 0 \text{ for any } d \in \mathbb{R}_+^n\}$.

Although problem (5.7) is a conic optimization problem, it is still difficult since determining whether $X \in \mathcal{C}_n^*$ or not is NP-hard [39]. A natural approach is to relax this problem to a more tractable optimization problem. Recall that the following inclusions hold:

$$\mathcal{C}_n^* \subseteq \mathcal{S}_+^n \cap \mathcal{N}^n \subseteq \mathcal{S}_+^n \subseteq \mathcal{S}_+^n + \mathcal{N}^n \subseteq \mathcal{C}_n.$$

By replacing $\mathcal{C}_n^*$ with $\mathcal{S}_+^n \cap \mathcal{N}^n$, one can obtain an SDP relaxation of (5.7):

$$\begin{aligned} \max\ & \langle ee^T, X\rangle \\ \text{s.t. } & \langle A+I, X\rangle = 1, \\ & X \in \mathcal{S}_+^n \cap \mathcal{N}^n. \end{aligned} \tag{5.8}$$

Solving this SDP is not as easy as it seems to be; in fact, we could not obtain a useful result of (5.8) after 6 hours of calculation using the state-of-the-art SDP solver Mosek for a random generalized problem when $n = 300$. We apply cutting-plane methods listed in Table 5.1 to (5.8). Note that since the adjacency matrix is entry-wise non-negative, i.e., $A \in \mathcal{N}^n$, we know that every feasible solution X of (5.8) satisfies $\mathrm{Tr}(X) = 1 - \langle A, X\rangle \leq 1$. This shows that Problem (5.8) naturally satisfies Assumption 5.1.1.

We tested methods in Table 5.1 on the Erdös-Rényi graphs $ER(n,p)$, randomly generated by Ahmadi et al. in [1], where n is the number of vertices and every pair of vertices has an edge with probability p. All experiments were performed with MATLAB 2018b on a Windows PC with an Intel(R) Core(TM) i7-6700 CPU running at 3.4 GHz and 16 GB of RAM. The LPs were solved using Gurobi Optimizer 8.0.0 [53] and the SOCPs and SDPs are solved using Mosek Optimizer 9.0 [6]. Similar to Section 5.2, we use the gap between the upper bounds of each method and the SDP bound obtained by (5.8),i.e., $\left|\frac{f^*-f_k}{f^*}\right| \times 100\%$, to evaluate methods in Table 5.1.

Figure 5.3 shows the result for an instance with $n = 250$ and $p = 0.8$. The x-axis is the number of iterations, and the y-axis is the gap between the upper bounds of each method and the SDP bound obtained by (5.8). As can be seen in this figure, the accuracy of CPDD is the worst among the four methods at each iteration. CPSDB achieves almost the same upper bounds as CPSDD and SDSOS, which shows that the proposed polyhedral approximation $\mathcal{SDB}_n$ is promising for obtaining a solution close to the non-polyhedral approximation $\mathcal{SDD}_n$ of $\mathcal{S}^n_+$. Although SDSOS adds an extra SOCP cut at every iteration and takes longer to solve, the accuracy of SDSOS does not seem to be affected and is not so different from the accuracy of CPSDD at each iteration.

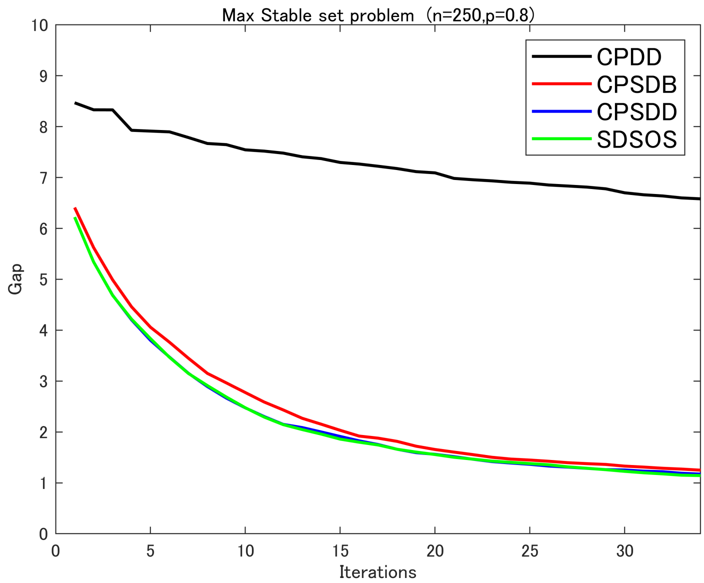


Figure 5.3: Relation between the number of iterations and the gap for a maximum stable set problem

Figure 5.4 shows the relation between the computation time and the gap of each method for the same instance. Although its accuracy is not necessarily the best at every iteration, it seems that CPSDB is the most efficient method. CPSDB attains an upper bound whose gap is 2 within 30 s, while CPSDD and SDSOS attain upper bounds whose gap is 4 after the same amount of time. The difference might come from that the subproblems of CPSDB are sparse LPs at earlier iterations and the computations are relatively cheaper than those of CPSDD and SDSOS whose subproblems are SOCPs.

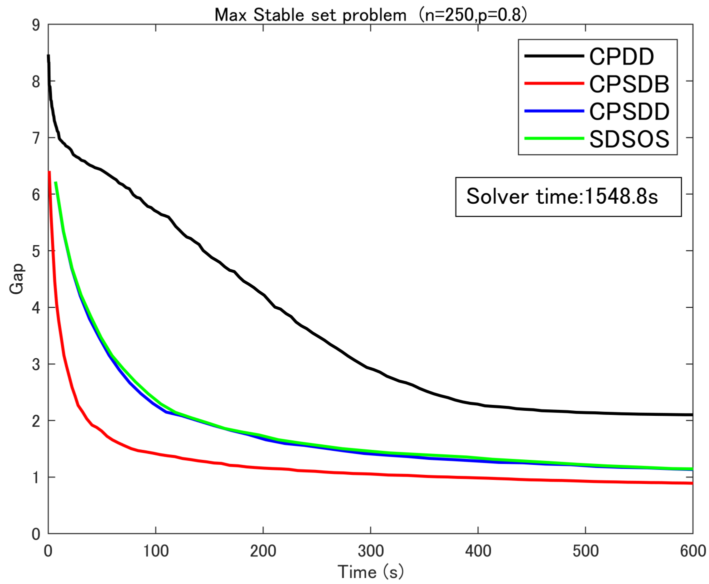


Figure 5.4: Relation between the computational time and the gap for the same maximum stable set problem

Table 5.3 and 5.4 give the bounds of iterative methods and the SDP bound for all the instances. In Table 5.3, the $\text{CPSDD}_0/\text{SDSOS}_0$ column shows the first upper bound obtained by CPSDD and SDSOS, i.e., the upper bound obtained by solving the same SOCP before adding any cutting-plane. The (5 min) and (10 min) columns of CPSDD (SDSOS) show the upper bounds obtained after 5 minutes and after 10 minutes of the CPSDD (SDSOS) computation, respectively. The SDP column shows the SDP bound obtained by solving (5.8).

Similarly, in Table 5.4, the CPDD_0 and CPSDB_0 columns show the first upper bounds obtained by CPDD and CPSDB, respectively, before adding any cutting-plane. The (5 min) and (10 min) columns of CPDD (CPSDB) show the upper bounds obtained after 5 minutes and after 10 minutes of the CPDD (CPSDB) computation, respectively.

Note that we failed to solve SDPs (5.8) for instances having $n = 300$ nodes within our time limit 20000s. In Table 5.3, the Value and Time (s) columns of SDP with $n = 300$ show the results obtained in [1] for these two instances, as a reference.

As can be seen in Table 5.3 and 5.4, for all instances, the values of $\text{CPSDD}_0/\text{SDSOS}_0$ are better than the values of CPSDB_0 and CPDD_0. These results correspond to the inclusion relationship of initial approximations (5.5). We can also see that the values of CPSDB_0 are almost the same as those of $\text{CPSDD}_0/\text{SDSOS}_0$ for all instances, while the values of CPDD_0 are much worse than others. For all instances, CPSDB seems to be significantly more efficient than all other methods. For example, for instance with $n = 250$ and $p = 0.3$, after 10 min of calculation, CPSDB obtained an upper bound of 73.24, while CPSDD and SDSOS got upper bounds greater than 90 and CPDD got a bound of more than 146.

At present, solving a large SDP, e.g., one with more than $n = 300$ nodes requires a significant amount of computational time. The cutting-plane method CPSDB with our polyhedral approximation $\mathcal{SDB}_n$ is a promising way of obtaining efficient upper bounds of such large SDPs in a moderate time.

Table 5.3: Upper bounds obtained by SDP and SOCP methods on $ER(n,p)$ graphs

n	p	$\text{CPSDD}_0/\text{SDSOS}_0$		CPSDD		SDSOS		SDP	
		Value	Time (s)	(5 min)	(10 min)	(5 min)	(10 min)	Value	Time (s)
150	0.3	105.70	0.95	38.91	37.02	40.97	37.38	20.44	105.46
150	0.8	31.78	1.00	10.07	9.66	9.70	9.31	6.00	110.63
200	0.3	140.47	3.14	70.48	55.52	75.46	61.31	23.73	549.63
200	0.8	40.92	3.14	12.10	11.29	12.17	11.38	6.45	497.55
250	0.3	176.25	6.60	115.41	93.81	119.67	99.99	26.78	1562.52
250	0.8	51.87	6.79	17.36	15.30	17.43	15.39	7.18	1553.63
300	0.3	210.32	13.05	160.42	138.60	162.77	143.12	(29.13)	(32300.60)
300	0.8	60.97	13.31	21.71	17.77	22.66	18.50	(7.65)	(20586.02)

Table 5.4: Upper bounds obtained by LP methods on the same $ER(n,p)$ graphs

n	p	CPDD_0		CPDD		CPSDB_0		CPSDB	
		Value	Time (s)	(5 min)	(10 min)	Value	Time (s)	(5 min)	(10 min)
150	0.3	117	0.06	76.76	67.51	107.29	0.24	36.80	35.12
150	0.8	46	0.05	13.70	12.71	32.76	0.28	9.51	9.06
200	0.3	157	0.1	113.28	104.07	142.25	0.52	55.07	48.18
200	0.8	54	0.11	17.39	16.07	42.14	0.57	11.58	11.00
250	0.3	194	0.17	154.75	146.20	178.30	0.84	91.88	73.24
250	0.8	68	0.17	28.02	22.26	53.22	1.00	14.76	13.57
300	0.3	230	0.26	183.89	174.02	212.97	1.29	133.83	110.95
300	0.8	78	0.24	47.87	32.28	62.47	1.36	18.11	16.05

5.3 Conclusion

In this chapter, we introduced a cutting-plane method for solving semidefinite optimization problems and described the vital role of approximations of $\mathcal{S}^n_+$ in this method. Approximations introduced in Chapter 3, including $\mathcal{DD}^*_n$, $\mathcal{SDD}^*_n$ and our approximation $\mathcal{SDB}^*_n$, were applied to the cutting-plane method for solving randomly generated instances of DNN problems and a semidefinite relaxation of the maximum stable set problem. The results of the numerical experiments showed that the cutting-plane method with our approximation $\mathcal{SDB}^*_n$ is more efficient than other methods (see Figure 5.2 and Figure 5.4); improving the efficiency of our method remains an important study issue.

Chapter 6

Conclusion and implications

6.1 Summary

Semidefinite optimization has wide applications in convex optimizations, combinatorial and nonconvex optimizations and control theory. The computational tractability of SDPs mainly comes from the fact that SDPs can be solved in polynomial time to any desired precision with interior-point methods. However, their computations become difficult when the size of the SDP becomes large. As an alternative class of methods to compensate for the weakness of interior-point methods, cutting-plane methods are able to obtain tightly approximated solutions of SDPs in a considerable amount of time. In this thesis, we focused on cutting-plane methods, which generate relaxations of SDPs and solve them as easily handled optimization problems, e.g., LPs and SOCPs. In particular, we focused on what impacts the initial relaxation problem, i.e., the approximations of the semidefinite cone. We constructed a series of tight and sparse polyhedral approximations of the semidefinite cone based on SD bases proposed by Tanaka and Yoshise [106]. Then we conducted theoretical analyses and evaluate some of the approximations of the semidefinite cone. Finally, we applied our proposed approximation of the semidefinite cone to a cutting plane method and performed numerical experiments on random DNN instances as well as maximum stable set problems. The numerical results showed the efficiency of the cutting plane method using our proposed approximation.

In Chapter 3, we explored the inclusive relation of several existing approximations of the semidefinite cone, including the set of matrices with factor width at most k, i.e., $\mathcal{FW}_n(k)$, the set of (resp., scaled) diagonally dominant matrices, i.e., $\mathcal{DD}_n$ (resp., $\mathcal{SDD}_n$), and their dual cones. Based on the concept of the SD basis, we proposed an expansion of SD bases with a parameter in Section 3.2, which gives an orthogonal basis of $\mathbb{S}^n$ on the boundary of $\mathcal{S}^n_+$. The conditions for generating an expansion different from the existing one are given in Proposition 3.2.3. Using the expanded SD bases, we proposed a new sparse polyhedral approximation $\mathcal{SDB}_n(\mathcal{H})$, which is controlled by a parameter set $\mathcal{H}$. As concluded in Corollary 3.2.7, we showed that the polyhedral approximation using our expanded SD bases contains the set of diagonally dominant matrices and is contained in the set of scaled diagonally dominant matrices, i.e., $\mathcal{DD}_n \subseteq \mathcal{SDB}_n(\mathcal{H}) \subseteq \mathcal{SDD}_n$ whenever $\{1, -1\} \subseteq \mathcal{H} \subseteq \mathbb{R}$. Moreover, it is proved in Theorem 3.2.6 that the set of scaled diagonally dominant matrices can be expressed using an infinite number of expanded SD bases, i.e., $\mathcal{SDB}_n(\mathbb{R}) = \mathcal{SDD}_n$. A practical method for calculating parameters for our proposed approximation $\mathcal{SDB}_n(\mathcal{H})$ is also presented in Section 3.2.3.

In Chapter 4, we evaluated the above approximations using the norm normalized distance, which calculates the maximum distance from a matrix in a given approximation to the semidefinite cone under the constraint that the value of the Frobenius norm is one. Unfortunately, we proved in Theorem 4.2.1 that the norm normalized distance from a set to the semidefinite cone, i.e., $\overline{\text{dist}}_F(\mathcal{S}, \mathcal{S}^n_+)$, has the same value whenever $\mathcal{SDD}^*_n \subseteq \mathcal{S} \subseteq \mathcal{DD}^*_n$. This result implies that the norm normalized distance is not sufficient to evaluate these approximations, possibly because the normalization using Frobenius norm is too strict that evens out some differences among these sets.

In Section 4.3, as a new measure to compensate for the weakness of that distance, we proposed the trace normalized distance ,i.e., $\overline{\text{dist}}_T(\cdot, \mathcal{S}^n_+)$, which has a weaker normalization constraint that the trace of a matrix is one. By using this measure, we showed that the trace normalized distance from $\mathcal{DD}^*_n$ to the semidefinite cone differs from the trace normalized distance from $\mathcal{SDD}^*_n$ to the semidefinite cone, i.e., $\overline{\text{dist}}_T(\mathcal{DD}^*_n, \mathcal{S}^n_+) = \frac{\sqrt{n}-1}{2}$ (Theorem 4.3.6) and $\overline{\text{dist}}_T(\mathcal{SDD}^*_n, \mathcal{S}^n_+) = \frac{n-2}{n}$ (Theorem 4.3.3).

Note that the trace normalized distance from the polyhedral cone $\mathcal{DD}^*_n$ to the semidefinite cone is calculated by finding the structures of the extreme points of $\mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid \text{Tr}(X) = 1\}$. Although our proposed approximation $\mathcal{SDB}^*_n(\mathcal{H})$ with a parameter set $\mathcal{H}$ is also a polyhedral cone, it is hard to explore all its extreme points. Then we tried another way to evaluate our proposed approximation in Section 4.4. We proposed a measure called the extreme point distance, i.e., $\underline{\text{Edist}}_T(\mathcal{DD}^*_n, \mathcal{S})$, which calculates the minimum distance between a set $\mathcal{S}$ and the extreme points of $\mathcal{DD}^*_n \cap \{X \in \mathbb{S}^n \mid \text{Tr}(X) = 1\}$. We numerically calculated this measure for $\mathcal{SDD}^*_n$ and $\mathcal{SDB}^*_n(\mathcal{H})$ with several $\mathcal{H}$, and showed that with a specific parameter set $\bar{\mathcal{H}}$, $\underline{\text{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDB}^*_n(\bar{\mathcal{H}}))$ stays very close to $\underline{\text{Edist}}_T(\mathcal{DD}^*_n, \mathcal{SDD}^*_n)$ for each n.

In Chapter 5, we introduced a cutting plane method for solving SDPs and conducted numerical experiments with different initial approximations of the semidefinite cone, including $\mathcal{DD}^*_n$, $\mathcal{SDD}^*_n$ and our proposed approximation $\mathcal{SDB}^*_n(\bar{\mathcal{H}})$ with a specific parameter set $\bar{\mathcal{H}}$. Experimental results indicated that the cutting plane method using our approximation

$\mathcal{SDB}_n^*(\bar{\mathcal{H}})$ is promising not only for random DNN problems but also for the maximum stable set problem.

6.2 Future direction

On expanded SD bases

One future direction is to utilize sparse patterns to generate specific approximations of the semidefinite cone using SD bases. For example, consider checking the positive semidefiniteness of a matrix that has elements only in certain rows/columns (e.g., with index set $\mathcal{I}$) and diagonal positions. Then we can reduce the number of bases in SD bases and only use matrices $(e_i+e_j)(e_i+e_j)^T$ with $i,j \in \mathcal{I}$ to construct specific inner and outer approximations of the semidefinite cone. The relation between sparsity patterns and SD bases is an exciting issue to be considered in the future.

As for the parameter α, which is used to generate matrices in expanded SD bases: $(e_i + \alpha e_j)(e_i + \alpha e_j)^T$, we developed a practical technique to calculate parameters that provide generally large inner approximations for the semidefinite cone. However, in practice, the parameter α is often problem-dependent. For example, in the cutting plane method for solving SDPs, a problem-dependent choice of the parameter set may lead to a specific initial approximation of the semidefinite cone, and give us a tighter initial bound for the optimal value. Accordingly, it is an attractive issue to explore the choice of parameters problem-dependently.

We may also consider increasing the number of vectors in the definition of the SD bases. The current SD bases are defined as a set of matrices $(e_i + e_j)(e_i + e_j)^T$. If we use three vectors, as in $(e_i + e_j + e_k)(e_i + e_j + e_k)^T$, we might obtain another inner approximation that remains relatively sparse when the dimension n is large. To construct an inner approximation, we need to generate C_n^3 base matrices like $(e_i + e_j + e_k)(e_i + e_j + e_k)^T$. One may investigate how to efficiently reduce the number of bases matrices while keeping the approximation tight. In the same manner as we expand the SD basis, we may expand $(e_i + e_j + e_k)(e_i + e_j + e_k)^T$ by using parameters α, β: $(e_i + \alpha e_j + \beta e_k)(e_i + \alpha e_j + \beta e_k)^T$. However, this expansion may be hard to control since there are two parameters. These issues may be interesting to discover in the future.

More applications of our proposed approximation should be explored in the future. For example, the proposed approximation $\mathcal{SDB}_n^*$ can be considered to be applied to the partial facial reduction technique [95]. In recent years, Tanaka and Yoshise [106] proposed an LP-based method to test copositivity of a matrix using SD bases. Gouveia et al. [51] developed an SOCP-based approximation scheme for completely positive and copositive optimization problems using the set of nonnegative scaled diagonally dominant matrices. We may investigate more applications of our proposed SD bases on copositive optimization.

On the evaluation of approximations using expanded SD bases

As for the evaluation of approximations, we also have some future directions. Note that the trace normalized distance from the polyhedral cone $\mathcal{DD}_n^*$ to the semidefinite cone is calculated by finding the structures of the extreme points of $\mathcal{DD}_n^* \cap \{X \in \mathbb{S}^n \mid \mathrm{Tr}(X) = 1\}$. Since our proposed approximation $\mathcal{SDB}_n^*(\mathcal{H})$ with a parameter set $\mathcal{H}$ is also a polyhedral cone, it will be an interesting but also challenging issue to explore all extreme points of $\mathcal{SDB}_n^*(\mathcal{H})$. By obtaining these extreme points, we can directly analyze the trace normalized distance from $\mathcal{SDB}_n^*(\mathcal{H})$ to the semidefinite cone: $\overline{\mathrm{dist}}_T(\mathcal{SDB}_n^*(\mathcal{H}), \mathcal{S}_+^n)$.

One may notice that in the proof of convergence of the cutting plane method in Section 5, i.e., the proof of Theorem 5.1.3, we used an argument which states that the Euclidean balls of radius $\frac{\epsilon}{2}$ centered at the points returned by the algorithm are contained in a ball of radius $R + \frac{\epsilon}{2}$ centered at the origin. Then we showed that the volume of non-overlapping balls centered at these points is smaller than the volume of the ball of radius $R + \frac{\epsilon}{2}$. Using this relation, the convergence rate of the algorithm is derived. In fact, for a given initial approximation $\mathcal{P}_0^n$ of the semidefinite cone, the balls centered at the points returned by the algorithm should lie in the set $\mathcal{P}_0^n \setminus \mathcal{S}_+^n$. By replacing the volume of the ball of radius $R + \frac{\epsilon}{2}$ using the volume of the Minkowski sum of $\mathcal{P}_0^n \setminus \mathcal{S}_+^n$ and a ball of radius $\frac{\epsilon}{2}$ centered at the origin, we may obtain a significantly tighter convergence rate. Hence, it would be very interesting to look into the relationship between the volume of $\mathcal{P}_0^n \setminus \mathcal{S}_+^n$ and the trace normalized distances $\overline{\mathrm{dist}}_T(\mathcal{P}_0^n, \mathcal{S}_+^n)$ in the future.

On generalizations of factor width

Also, there is a future direction to focus on the factor width k of a matrix. The cone of matrices with factor width at most k, i.e., $\mathcal{FW}_n(k)$, provides an approximation of the semidefinite cone. As has been illustrated in Figure 3.1, by considering a larger width $k > 2$, we may obtain a more considerable inner approximation of the semidefinite cone, although it would not be polyhedral or even characterized by using SOCP constraints. In fact, Fawzi [42] showed that 3×3 positive semidefinite cone does not admit any second-order cone representation. Checking whether a matrix is in $\mathcal{FW}_n(k)$ or its dual cone $\mathcal{S}^{n,k}$ requires to solve a semidefinite optimization problem with C_n^k semidefinite constraints of size k, which seems to be not efficient for $k \geq 3$. Thus in practice, $\mathcal{FW}_n(k)$ and $\mathcal{S}^{n,k}$ are used to solve SDPs by setting $k \leq 2$. Finding efficient ways to solve optimization problems over $\mathcal{FW}_n(k)$ with $k \geq 3$ might be an exciting challenge.

In a recent paper, Zheng et al. [124] proposed an extension of the factor width 2 matrices, i.e., the block factor-width-two matrices, using the matrix block partition, which aims to alleviate the deficiency mentioned above. By using a matrix partition $\alpha = \{k_1, \ldots, k_p\}$, a matrix $A \in \mathbb{R}^{n\times n}$ can be partitioned into small block matrices $A_{i,j} \in \mathbb{R}^{k_i\times k_j}$. Checking whether a matrix is in the set of block factor-width-two matrices with partition α requires only $\frac{p(p-1)}{2}$ semidefinite constraints with size $k_1, \ldots, k_p$. It is an interesting issue to investigate more on the relation between matrix partition and the set of factor width k matrices.

Bibliography

[1] Amir Ali Ahmadi, Sanjeeb Dash, and Georgina Hall. Optimization over structured subsets of positive semidefinite matrices via column generation. *Discrete Optimization*, 24:129–151, 2017.

[2] Amir Ali Ahmadi and Anirudha Majumdar. Dsos and sdsos optimization: more tractable alternatives to sum of squares and semidefinite optimization. *SIAM Journal on Applied Algebra and Geometry*, 3:193–230, 2019.

[3] Farid Alizadeh. *Combinatorial Optimization with Interior Point Methods and Semi-Definite Matrices*. PhD thesis, University of Minnesota, USA, 1992. UMI Order No. GAX92-07776.

[4] Farid Alizadeh. Interior point methods in semidefinite programming with applications to combinatorial optimization. *SIAM Journal on Optimization*, 5(1):13–51, 1995.

[5] Martin S Andersen, Joachim Dahl, and Lieven Vandenberghe. Implementation of nonsymmetric interior-point methods for linear optimization over sparse matrix cones. *Mathematical Programming Computation*, 2(3):167–201, 2010.

[6] MOSEK ApS. *The MOSEK optimization toolbox for MATLAB manual. Version 9.0.*, 2019 [Accessed: 2021-3-12].

[7] Naohiko Arima, Sunyoung Kim, and Masakazu Kojima. A quadratically constrained quadratic optimization model for completely positive cone programming. *SIAM Journal on Optimization*, 23(4):2320–2340, 2013.

[8] Naohiko Arima, Sunyoung Kim, Masakazu Kojima, and Kim-Chuan Toh. A robust Lagrangian-DNN method for a class of quadratic optimization problems. *Computational Optimization and Applications*, 66(3):453–479, 2017.

[9] Naohiko Arima, Sunyoung Kim, Masakazu Kojima, and Kim-Chuan Toh. Lagrangian-conic relaxations, part i: A unified framework and its applications to quadratic optimization problems. *Pacific Journal of Optimization*, 14(1):161–192, 2018.

[10] George Barker and David Carlson. Cones of diagonally dominant matrices. *Pacific Journal of Mathematics*, 57(1):15–32, 1975.

[11] Heinz Bauer. Minimalstellen von funktionen und extremalpunkte. *Archiv der Mathematik*, 9:389–393, 1958.

[12] Abraham Berman and Robert J. Plemmons. *Nonnegative Matrices in the Mathematical Sciences*. Society for Industrial and Applied Mathematics, 1994.

[13] Abraham Berman and Naomi Shaked-Monderer. *Completely Positive Matrices*. WORLD SCIENTIFIC, 2003.

[14] Dimitri Bertsekas. Nonlinear programming. *Journal of the Operational Research Society*, 48(3):334–334, 1997.

[15] Dimitri Bertsekas. *Convex optimization theory.* Athena Scientific Belmont, 2009.

[16] Dimitri Bertsekas, Angelia Nedic, and Asuman Ozdaglar. *Convex analysis and optimization*, volume 1. Athena Scientific, 2003.

[17] Dimitris Bertsimas and Ryan Cory-Wright. On polyhedral and second-order cone decompositions of semidefinite optimization problems. *Operations Research Letters*, 48(1):78–85, 2020.

[18] Li Bishan, Li Lei, Masunori Harada, Hiroshi Niki, and Michael J. Tsatsomeros. An iterative criterion for h-matrices. *Linear Algebra and its Applications*, 271(1):179–190, 1998.

[19] Robert G. Bland, Donald Goldfarb, and Michael J. Todd. Feature article—the ellipsoid method: A survey. *Operations Research*, 29(6):1039–1091, 1981.

[20] Grigoriy Blekherman, Santanu S. Dey, Marco Molinaro, and Shengding Sun. Sparse psd approximation of the psd cone. *Mathematical Programming*, 2020.

[21] Grigoriy Blekherman, Santanu S Dey, Kevin Shu, and Shengding Sun. Hyperbolic relaxation of k-locally positive semidefinite matrices. *arXiv preprint arXiv:2012.04031*, 2020.

[22] Grigoriy Blekherman, Pablo A. Parrilo, and Rekha R. Thomas. *Semidefinite Optimization and Convex Algebraic Geometry.* Society for Industrial and Applied Mathematics, Philadelphia, PA, 2012.

[23] Erik G. Boman, Doron Chen, Ojas Parekh, and Sivan Toledo. On factor width and symmetric h-matrices. *Linear Algebra and its Applications*, 405:239–248, 2005.

[24] Jon M. Borwein and Henry Wolkowicz. Facial reduction for a cone-convex programming problem. *Journal of the Australian Mathematical Society. Series A. Pure Mathematics and Statistics*, 30(3):369–380, 1981.

[25] Stephen Boyd, Laurent El Ghaoui, Eric Feron, and Venkataramanan Balakrishnan. *Linear Matrix Inequalities in System and Control Theory.* Society for Industrial and Applied Mathematics, 1994.

[26] Stephen Boyd and Lieven Vandenberghe. *Convex optimization.* Cambridge university press, 2004.

[27] Samuel Burer. On the copositive representation of binary and continuous nonconvex quadratic programs. *Mathematical Programming*, 120(2):479–495, 2009.

[28] Samuel Burer and Renato D. C. Monteiro. A projected gradient algorithm for solving the maxcut sdp relaxation. *Optimization Methods and Software*, 15(3-4):175–200, 2001.

[29] Samuel Burer and Renato DC Monteiro. A nonlinear programming algorithm for solving semidefinite programs via low-rank factorization. *Mathematical Programming*, 95(2):329–357, 2003.

[30] Samuel Burer and Renato DC Monteiro. Local minima and convergence in low-rank semidefinite programming. *Mathematical programming*, 103(3):427–444, 2005.

[31] Sergei Chubanov. A polynomial projection algorithm for linear feasibility problems. *Mathematical Programming*, 153:687–713, 2015.

[32] IBM ILOG Cplex. V20. 1: User's manual for cplex, 2020, [Accessed: 2021-9-1].

[33] George Dantzig. Programming of interdependent activities: II mathematical model. *Econometrica*, 17(3/4):200–211, 1949.

[34] George Dantzig, Ray Fulkerson, and Selmer Johnson. Solution of a large-scale traveling-salesman problem. *Journal of the Operations Research Society of America*, 2(4):393–410, 1954.

[35] George Dantzig, Ray Fulkerson, and Selmer Johnson. On a linear-programming, combinatorial approach to the traveling-salesman problem. *Operations Research*, 7(1):58–66, 1959.

[36] Etienne de Klerk. *Aspects of semidefinite programming: interior point algorithms and selected applications*, volume 65. Springer Science & Business Media, 2002.

[37] Etienne de Klerk. Exploiting special structure in semidefinite programming: A survey of theory and applications. *European Journal of Operational Research*, 201(1):1–10, 2010.

[38] Etienne de Klerk and Dmitrii V. Pasechnik. Approximation of the stability number of a graph via copositive programming. *SIAM Journal on Optimization*, 12(4):875–892, 2002.

[39] Peter J. C. Dickinson and Luuk Gijben. On the computational complexity of membership problems for the completely positive cone and its dual. *Computational Optimization and Applications*, 57(2):403–415, 2014.

[40] Peter J.C. Dickinson. Geometry of the copositive and completely positive cones. *Journal of Mathematical Analysis and Applications*, 380(1):377–395, 2011.

[41] Mirjam Dür. Copositive programming – a survey. In Moritz Diehl, Francois Glineur, Elias Jarlebring, and Wim Michiels, editors, *Recent Advances in Optimization and its Applications in Engineering*, pages 3–20, Berlin, Heidelberg, 2010. Springer Berlin Heidelberg.

[42] Hamza Fawzi. On representing the positive semidefinite cone using the second-order cone. *Mathematical Programming*, 175(1):109–118, 2019.

[43] Hamza Fawzi. On polyhedral approximations of the positive semidefinite cone. *Mathematics of Operations Research*, 2021.

[44] Robert M Freund. On the behavior of the homogeneous self-dual model for conic convex optimization. *Mathematical programming*, 106(3):527–545, 2006.

[45] Robert M. Freund, Paul Grigas, and Rahul Mazumder. An extended frank–wolfe method with "in-face" directions, and its application to low-rank matrix completion. *SIAM Journal on Optimization*, 27(1):319–346, 2017.

[46] Mituhiro Fukuda, Masakazu Kojima, Kazuo Murota, and Kazuhide Nakata. Exploiting sparsity in semidefinite programming via matrix completion i: General framework. *SIAM Journal on Optimization*, 11(3):647–674, 2001.

[47] S. Gerschgorin. Uber die abgrenzung der eigenwerte einer matrix. *lzv. Akad. Nauk. USSR. Otd. Fiz-Mat. Nauk*, 7:749–754, 1931.

[48] Michel X. Goemans and David P. Williamson. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *J. ACM*, 42(6):1115–1145, November 1995.

[49] Ralph E. Gomory. Outline of an algorithm for integer solutions to linear programs. *Bulletin of the American Mathematical Society*, 64(5):275 – 278, 1958.

[50] Clovis C. Gonzaga. Path-following methods for linear programming. *SIAM Review*, 34(2):167–224, 1992.

[51] João Gouveia, Ting Kei Pong, and Mina Saee. Inner approximating the completely positive cone via the cone of scaled diagonally dominant matrices. *Journal of Global Optimization*, 76(2):383–405, 2020.

[52] Robert Grone, Charles R Johnson, Eduardo M Sá, and Henry Wolkowicz. Positive definite completions of partial hermitian matrices. *Linear Algebra and its Applications*, 58:109–124, 1984.

[53] Gurobi Optimization, LLC. Gurobi Optimizer Reference Manual, 2021, [Accessed: 2021-8-15].

[54] Elad Hazan. Sparse approximate solutions to semidefinite programs. In *Latin American symposium on theoretical informatics*, pages 306–316. Springer, 2008.

[55] Christoph Helmberg. Semidefinite programming for combinatorial optimization, 2000.

[56] Christoph Helmberg. Semidefinite programming. *European Journal of Operational Research*, 137(3):461–482, 2002.

[57] Christoph Helmberg, Franz Rendl, and Robert Weismantel. Quadratic knapsack relaxations using cutting planes and semidefinite programming. In *International Conference on Integer Programming and Combinatorial Optimization*, pages 175–189. Springer, 1996.

[58] Christoph Helmberg, Franz Rendl, and Robert Weismantel. A semidefinite programming approach to the quadratic knapsack problem. *Journal of combinatorial optimization*, 4(2):197–215, 2000.

[59] Roger A. Horn and Charles R. Johnson. *Matrix Analysis*. Cambridge University Press, USA, 2nd edition, 2012.

[60] Hao Hu, Renata Sotirov, and Henry Wolkowicz. Facial reduction for symmetry reduced semidefinite programs. *arXiv preprint arXiv:1912.10245*, 2019.

[61] Naonori Kakimura. A direct proof for the matrix decomposition of chordal-structured positive semidefinite matrices. *Linear Algebra and its Applications*, 433(4):819–823, 2010.

[62] Shin-ichi Kanoh and Akiko Yoshise. Centering admm for the semidefinite relaxation of the qap. *arXiv preprint arXiv:2001.05739*, 2020.

[63] Stefan E. Karisch and Franz Rendl. Semidefinite programming and graph equipartition. In *IN TOPICS IN SEMIDEFINITE AND INTERIOR-POINT METHODS*, pages 77–95. AMS, 1998.

[64] Narendra Karmarkar. A new polynomial-time algorithm for linear programming. *Combinatorica*, 4:373–395, 1984.

[65] J. E. Kelley, Jr. The cutting-plane method for solving convex programs. *Journal of the Society for Industrial and Applied Mathematics*, 8(4):703–712, 1960.

[66] Leonid Genrikhovich Khachiyan. A polynomial algorithm in linear programming. In *Doklady Akademii Nauk*, volume 244, pages 1093–1096. Russian Academy of Sciences, 1979.

[67] Sunyoung Kim and Masakazu Kojima. Exact Solutions of Some Nonconvex Quadratic Optimization Problems via SDP and SOCP Relaxations. *Computational Optimization and Applications*, 26(2):143–154, 2003.

[68] Sunyoung Kim, Masakazu Kojima, and Kim-Chuan Toh. A Lagrangian–DNN relaxation: a fast method for computing tight lower bounds for a class of quadratic optimization problems. *Mathematical Programming*, 156(1):161–187, 2016.

[69] Victor Klee and George J Minty. How good is the simplex algorithm. *Inequalities*, 3(3):159–175, 1972.

[70] Ken Kobayashi and Yuich Takano. A branch-and-cut algorithm for solving mixed-integer semidefinite optimization problems. *Computational Optimization and Applications*, 75(2):493–513, 2020.

[71] Masakazu Kojima, Shinji Mizuno, and Akiko Yoshise. A primal-dual interior point algorithm for linear programming. In *Progress in mathematical programming*, pages 29–47. Springer, 1989.

[72] Hiroshi Konno, Jun-ya Gotoh, Takeaki Uno, and Atsushi Yuki. A cutting plane algorithm for semi-definite programming problems with applications to failure discriminant analysis. *J. Comput. Appl. Math.*, 146(1):141–154, September 2002.

[73] Kartik Krishnan and John E Mitchell. *A linear programming approach to semidefinite programming problems*. PhD thesis, Citeseer, 2002.

[74] Kartik Krishnan and John E Mitchell. A Semidefinite Programming Based Polyhedral Cut and Price Approach for the Maxcut Problem. *Computational Optimization and Applications*, 33(1):51–71, 2006.

[75] Kartik Krishnan and John E. Mitchell. A unifying framework for several cutting plane methods for semidefinite programming. *Optimization Methods and Software*, 21(1):57–74, 2006.

[76] Martin Kružík. Bauer's maximum principle and hulls of sets. *Calculus of Variations and Partial Differential Equations*, 11(3):321–332, 2000.

[77] Jean B. Lasserre. An explicit exact sdp relaxation for nonlinear 0-1 programs. In *Proceedings of the 8th International IPCO Conference on Integer Programming and Combinatorial Optimization*, page 293–303, Berlin, Heidelberg, 2001. Springer-Verlag.

[78] Jean B. Lasserre. A quick proof for the volume of n-balls. *The American Mathematical Monthly*, 108(8):768–769, 2001.

[79] Monique Laurent and Frank Vallentin. Semidefinite optimization. Lecture Notes, available at `https://homepages.cwi.nl/~monique/master_SDP_2016.pdf`, 2016, [Accessed: 2021-7-5].

[80] Bruno F Lourenço, Tomonari Kitahara, Masakazu Muramatsu, and Takashi Tsuchiya. An extension of chubanov's algorithm to symmetric cones. *Mathematical Programming*, 173(1):117–149, 2019.

[81] David G Luenberger and Yinyu Ye. *Linear and nonlinear programming*, volume 228. Springer, fourth edition edition, 2016.

[82] Ramtin Madani, Abdulrahman Kalbat, and Javad Lavaei. Admm for sparse semidefinite programming with applications to optimal power flow problem. In *2015 54th IEEE Conference on Decision and Control (CDC)*, pages 5932–5939, 2015.

[83] Anirudha Majumdar, Georgina Hall, and Amir Ali Ahmadi. Recent scalability improvements for semidefinite programming with applications in machine learning, control, and robotics. *Annual Review of Control, Robotics, and Autonomous Systems*, 3(1):331–360, 2020.

[84] Kevin A McShane, Clyde L Monma, and David Shanno. An implementation of a primal-dual interior point method for linear programming. *ORSA Journal on computing*, 1(2):70–83, 1989.

[85] Nimrod Megiddo. Pathways to the optimal set in linear programming. In *Progress in mathematical programming*, pages 131–158. Springer, 1989.

[86] Hermann Minkowski. *Geometrie der zahlen.* Teubner, Leipzig: B, G, 1896.

[87] Renato DC Monteiro and Ilan Adler. Interior path following primal-dual algorithms. part i: Linear programming. *Mathematical programming*, 44(1):27–41, 1989.

[88] Katta G Murty and Santosh N Kabadi. Some NP-complete problems in quadratic and nonlinear programming. *Mathematical Programming*, 39(2):117–129, 1987.

[89] Almir Mutapcic and Stephen Boyd. Cutting-set methods for robust convex optimization with pessimizing oracles. *Optimization Methods and Software*, 24(3):381–406, 2009.

[90] Yurii Nesterov and Arkadii Nemirovski. *Interior-point polynomial algorithms in convex programming.* SIAM, 1994.

[91] Danilo Elias Oliveira, Henry Wolkowicz, and Yangyang Xu. Admm for the sdp relaxation of the qap. *Mathematical Programming Computation*, 10(4):631–658, 2018.

[92] Pablo A. Parrilo and Sanjay Lall. Semidefinite programming relaxations and algebraic optimization in control. *European Journal of Control*, 9(2):307–321, 2003.

[93] Javier Pena and Negar Soheili. Solving conic systems via projection and rescaling. *Mathematical Programming*, 166(1):87–111, 2017.

[94] Frank Permenter and Pablo A. Parrilo. Basis selection for sos programs via facial reduction and polyhedral approximations. In *53rd IEEE Conference on Decision and Control*, pages 6615–6620, 2014.

[95] Frank Permenter and Pablo A. Parrilo. Partial facial reduction: simplified, equivalent sdps via approximations of the psd cone. *Mathematical Programming*, 171:1–54, 2018.

[96] Frank Noble Permenter. *Reduction methods in semidefinite and conic optimization.* PhD thesis, Massachusetts Institute of Technology, 2017.

[97] James Renegar. *A Mathematical View of Interior-Point Methods in Convex Optimization.* Society for Industrial and Applied Mathematics, 2001.

[98] James Renegar. Accelerated first-order methods for hyperbolic programming. *Mathematical Programming*, 173(1):1–35, 2019.

[99] Ralph Tyrell Rockafellar. *Convex Analysis:.* Princeton University Press, 2015.

[100] Kees Roos. An improved version of chubanov's method for solving a homogeneous feasibility problem. *Optimization Methods and Software*, 33(1):26–44, 2018.

[101] Alexander Schrijver. A comparison of the delsarte and lovász bounds. *IEEE Transactions on Information Theory*, 25(4):425–429, 1979.

[102] Alexander Schrijver. *Theory of Linear and Integer Programming.* John Wiley & Sons, Inc., USA, 1986.

[103] Alexander Schrijver. *Combinatorial optimization: polyhedra and efficiency*, volume 24. Springer Science & Business Media, 2003.

[104] Naum Z Shor. Cut-off method with space extension in convex programming problems. *Cybernetics*, 13(1):94–96, 1977.

[105] Jos F. Sturm. Using sedumi 1.02, a matlab toolbox for optimization over symmetric cones. *Optimization Methods and Software*, 11(1-4):625–653, 1999.

[106] Akihiro Tanaka and Akiko Yoshise. LP-based tractable subcones of the semidefinite plus nonnegative cone. *Annals of Operations Research*, 265:155–182, 2018.

[107] Michael J. Todd. Potential-reduction methods in mathematical programming. *Mathematical Programming*, 76:3–45, 1997.

[108] Michael J. Todd. Semidefinite optimization. *Acta Numerica*, 10(515-560):126, 2001.

[109] Michael J. Todd. The many facets of linear programming. *Mathematical programming*, 91(3):417–436, 2002.

[110] Kim-Chuan Toh, Michael J. Todd, and Reha H. Tütüncü. Sdpt3 — a matlab software package for semidefinite programming, version 1.3. *Optimization Methods and Software*, 11(1-4):545–581, 1999.

[111] Lieven Vandenberghe and Stephen Boyd. Semidefinite programming. *SIAM Review*, 38(1):49–95, 1996.

[112] Lieven Vandenberghe and Stephen Boyd. Applications of semidefinite programming. *Applied Numerical Mathematics*, 29(3):283–299, 1999. Proceedings of the Stieltjes Workshop on High Performance Optimization Techniques.

[113] Hayato Waki and Masakazu Muramatsu. Facial Reduction Algorithms for Conic Optimization Problems. *Journal of Optimization Theory and Applications*, 158(1):188–215, 2013.

[114] Yuzhu Wang, Akihiro Tanaka, and Akiko Yoshise. Polyhedral approximations of the semidefinite cone and their application. *Computational Optimization and Applications*, 78:893–913, 2021.

[115] Yuzhu Wang and Akiko Yoshise. Evaluating approximations of the semidefinite cone with trace normalized distance. *arXiv preprint arXiv:2105.13579*, 2021.

[116] Zaiwen Wen, Donald Goldfarb, and Wotao Yin. Alternating direction augmented lagrangian methods for semidefinite programming. *Mathematical Programming Computation*, 2(3-4):203–230, 2010.

[117] Hermann Weyl. Elementare theorie der konvexen polyeder. *Commentarii Mathematici Helvetici*, 7:290–306, 1934.

[118] Henry Wolkowicz, Romesh Saigal, and Lieven Vandenberghe. *Handbook of semidefinite programming: theory, algorithms, and applications*, volume 27. Springer Science & Business Media, 2012.

[119] Stephen J. Wright. *Primal-Dual Interior-Point Methods*. Society for Industrial and Applied Mathematics, 1997.

[120] Makoto Yamashita, Katsuki Fujisawa, and Masakazu Kojima. Implementation and evaluation of sdpa 6.0 (semidefinite programming algorithm 6.0). *Optimization Methods and Software*, 18(4):491–505, 2003.

[121] Akiko Yoshise and Yasuaki Matsukawa. On optimization over the doubly nonnegative cone. In *2010 IEEE International Symposium on Computer-Aided Control System Design*, pages 13–18, 2010.

[122] David Berkovich Yudin and Arkadii Nemirovski. Informational complexity and efficient methods for the solution of convex extremal problems. *Matekon*, 13(2):22–45, 1976.

[123] Yang Zheng, Giovanni Fantuzzi, Antonis Papachristodoulou, Paul Goulart, and Andrew Wynn. Chordal decomposition in operator-splitting methods for sparse semidefinite programs. *Mathematical Programming*, 180(1):489–532, 2020.

[124] Yang Zheng, A. Sootla, and A. Papachristodoulou. Block factor-width-two matrices and their applications to semidefinite and sum-of-squares optimization. *ArXiv*, abs/1909.11076, 2019.

[125] Yuzixuan Zhu, Gábor Pataki, and Quoc Tran-Dinh. Sieve-sdp: a simple facial reduction algorithm to preprocess semidefinite programs. *Mathematical Programming Computation*, 11(3):503–586, 2019.