ON OUTER APPROXIMATIONS OF COPOSITIVE FORMULATIONS OF VARIOUS NONCONVEX OPTIMIZATION PROBLEMS

by

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Koç University

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This is to certify that I have examined this copy of a doctoral dissertation by

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To my beloved life partner

ABSTRACT

Copositive optimization is linear optimization over the convex cone of copositive or completely positive matrices. The term “copositive programming” was first introduced in 2000. In 2009, Burer showed that mixed binary quadratic optimization problems (MBQP), which comprises a rather large class of nonconvex and combinatorial problems, can be equivalently reformulated as a copositive optimization problem. This seminal work has greatly increased the interest in copositive optimization.

It is not surprising, however, that since many combinatorial and nonconvex optimization problems can be reformulated as a copositive optimization problem, copositive programs are also NP-hard in general. The difficulty in the reformulation is entirely due to the conic constraint. For this reason, many researchers have proposed outer approximation hierarchies to the intractable completely positive cone. These approximation hierarchies are composed of a sequence of tractable cones that yield increasingly better approximations of the completely positive cone and are exact in the limit.

By replacing the intractable cone by outer approximations in the copositive formulation of nonconvex and NP-hard minimization (resp. maximization) problems, a sequence of increasingly tighter lower (upper) bounds can be obtained for the original problem. This provides opportunities to obtain near-optimal solutions and improve the effectiveness of the algorithms for solving the original problem.

In this thesis, we study outer approximations of the copositive reformulations of three classes of nonconvex and NP-hard optimization problems. We first study the class of mixed binary programs (MBPs). We compare the lower bounds arising from

outer polyhedral approximations to the lower bound provided by the linear programming (LP) relaxation and establish that the lower bounds due to outer approximations are at least as good as that of LP relaxation. We establish various necessary or sufficient conditions under which the lower bound arising from the outer approximations matches that from the LP relaxation. Our results illustrate the weaknesses of polyhedral approximations. On the other hand, we show that the non-polyhedral doubly nonnegative (DNN) approximations, in general, yield tighter lower bounds.

Secondly, we focus on the specific 0-1 knapsack problem (KP) in the class of MBPs. We study two different copositive formulations of the knapsack and compare the upper bounds arising from outer polyhedral approximations to the upper bound provided by the LP relaxation of (KP). We prove that upper bounds obtained from outer polyhedral approximations actually coincide with the upper bound provided by the LP relaxation until at least a certain and fairly large level of the hierarchy. On the other hand, we establish that if the LP relaxation has a non-integer unique solution, then the DNN relaxation gives a strictly better upper bound than the LP relaxation.

Finally, we consider the standard quadratic programs (StQP) and investigate the instances of (StQP) for which the DNN relaxation is exact. We establish a complete algebraic characterization of the (StQP) instances that admit an exact DNN relaxation. We explicitly identify three different subsets of such (StQP) instances. Furthermore, we propose a recipe for constructing instances of (StQP) with an exact DNN relaxation.

In summary, our results reveal that outer polyhedral approximations, in general, yield weak bounds for (MBP) and for the specific 0-1 knapsack problem, whereas doubly nonnegative relaxations usually give rise to tighter lower bounds.

ÖZETÇE

Kopozitif eniyileme, dışbükey kopozitif veya tamamen pozitif koni üzerinde tanımlanan doğrusal eniyileme problemidir. “Kopozitif programlama” terimi ilk defa 2000 yılında ortaya atılmıştır. Daha sonra, Burer 2009 yılında kombinatoryal ve konveks olmayan problemlerin olduça geniş bir sınıfı olan karma ikili ikinci dereceden eniyileme problemlerinin bir kopozitif eniyileme problemi olarak formule edilebileceğini göstermiştir. Bu önemli çalışma, kopozitif programlama problemlerine olan ilgiyi önemli ölçüde arttırmıştır.

Ne var ki, kombinatoryal ve konveks olmayan birçok problemin bir kopozitif eniyileme problemine denk olması sebebiyle kopozitif formulasyonların da genel itibarıyla NP-zor olması şaşırtıcı değildir. Buradaki zorluk tam olarak konik kısıttan kaynaklanmaktadır. Bu sebeple birçok araştırmacı zorlu olan tamamen pozitif koniye kolay konilerden oluşan dıştan yaklaşıklama hiyerarşileri önermiştir. Bu yaklaşıklama hiyerarşilerinin temel prensibi, hiyerarşi seviyesi arttıkça tamamen pozitif koniyi daha iyi yaklaşıklayan ve limitte ona eşit olan bir koni dizisi üretmeye dayanmaktadır.

Konveks olmayan ve NP-zor birçok enküçükleme (enbüyükleme) probleminin kopozitif formulasyonundaki zorlu konik kısıt dıştan yaklaşımlar ile değiştirilerek problem için gittikçe sıkılaşan alt (üst) sınırlar elde edilebilmektedir. Bu durum, asıl problem için en iyi çözüme yakın çözümler elde etmek ve problemi çözmeye çalışan algoritmalar geliştirmek açısından fırsatlar sunmaktadır.

Bu tezde, üç farklı konveks olmayan ve NP-zor problem sınıfının kopozitif formulasyonlarının dış yaklaşıklamaları incelenmiştir. Öncelikle karma ikili tamsayı problemleri (MBP) ele alınmıştır. Bu problemde dış yaklaşımlardan elde edilen alt

sınırlar, problemin doğrusal programlama (LP) gevşetmesinden elde edilen alt sınır ile karşılaştırılmış ve bu alt sınırların en az LP gevşetmeden elde edilen alt sınır kadar iyi olacağı ortaya konmuştur. Bu sonuç olumlu gözükmekle birlikte, çok yüzlü dış yaklaşımlardan elde edilen alt sınırların belli bir seviyeye kadar iyileşmeyeceğini gösteren yeterli ya da gerekli koşullar ortaya konmuştur. Diğer yandan iki kat negatif olmayan (DNN) gevşetmelerin daha iyi alt sınırlar verdiğine yönelik bulgular elde edilmiştir.

İkinci olarak (MBP) sınıfındaki özel bir problem olan 0-1 sırt çantası problemi (KP) incelenmiştir. Sırt çantası probleminin iki farklı kopozitif formulasyonu çalışılmış ve çok yüzlü dış yaklaşımlardan elde edilen üst sınırlar LP gevşetmeden elde edilen üst sınırlar ile kıyaslanmıştır. Çok yüzlü dış yaklaşımlardan elde edilen üst sınırların LP gevşetmeden elde edilen üst sınır ile en azından belirli ve oldukça yüksek bir seviyeye kadar aynı alt sınırı vereceği kanıtlanmıştır. Diğer yandan, problemin LP gevşetmesinin tek ve tam sayı olmayan bir en iyi çözümü olması durumunda, DNN gevşetmenin LP gevşetmeden kesinlikle daha iyi alt sınır verdiği ortaya konmuştur.

Son olarak standart ikinci dereceden eniyileme probleminin (StQP) DNN gevşetmesinin tam (*exact*) olduğu örnekler incelenmiştir. DNN gevşetmenin tam olduğu örnekler için cebirsel bir karakterizasyon verilmiştir. DNN gevşetmenin tam olduğu örneklerin kümesi için üç farklı alt küme belirlenmiştir. Bu alt kümelerin her birindeki üyelik problemi polinom zamanda çözülebilmektedir. Ek olarak, DNN gevşetmenin tam olduğu (StQP) örneklerini inşa edebilmek için bir reçete sunulmaktadır.

Özetle, sonuçlarımız genel itibariyle çok yüzlü yaklaşımların (MBP) problemi ve 0-1 sırt çantası problemi için zayıf alt sınırlar verdiğine işaret etmekle birlikte, iki kat negatif olmayan gevşetmenin daha sıkı alt sınırlar verdiğine işaret etmektedir.

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NOMENCLATURE

$\mathbb{R}^n$	n-dimensional Euclidean space
$\mathbb{R}^n_+$	Set of n-dimensional nonnegative real vectors (Nonnegative orthant)
$\mathbb{Q}^n$	Set of n-dimensional rational vectors
$\mathbb{N}^n$	Set of n-dimensional nonnegative integer vectors
$\mathcal{S}^n$	Set of n-dimensional real symmetric matrices
$\mathcal{N}$	Cone of entrywise nonnegative matrices
$\mathcal{PSD}$	Cone of positive semidefinite matrices
$\mathcal{CP}$	Cone of completely positive matrices
$\mathcal{COP}$	Cone of copositive matrices
$\mathcal{DN}$	Cone of doubly nonnegative matrices ($\mathcal{PSD} \cap \mathcal{N}$)
$\mathcal{SPN}$	The dual cone of $\mathcal{DN}$ ($\mathcal{PSD} + \mathcal{N}$)
$\langle \cdot, \cdot \rangle$	Inner product
e	Vector of all ones
e_i	i-th unit vector
E	Matrix of all ones
E_{ij}	The symmetric matrix $1/2(e_i e_j^T + e_j e_i^T)$
$\text{Diag}(\cdot)$	Diagonal matrix with a specified vector
$\text{diag}(\cdot)$	Vector obtained from the diagonal entries of a given matrix

Nomenclature *(continued)*

(MBQP)	Mixed binary quadratic optimization problem
(MBP)	Mixed binary integer optimization problem
(KP)	0-1 Knapsack problem
(StQP)	Standard quadratic optimization problem
Rel(MBQP)	Continuous relaxation of (MBQP)
Rel(MBP)	LP relaxation of (MBP)
Rel(KP)	LP relaxation of (KP)
(MBQP-CP)	Copositive reformulation of (MBQP)
(MBP-CP)	Copositive reformulation of (MBP)
$(\text{KP-CP})^1$	First copositive reformulation of (KP)
$(\text{KP-CP})^2$	Second copositive reformulation of (KP)
$(\text{Out})_r$	r-th level outer approximation of the related copositive program
$(\text{Out})_r^1$	r-th level outer approximation of $(\text{KP-CP})^1$
$(\text{Out})_r^2$	r-th level outer approximation of $(\text{KP-CP})^2$
(DN)	Doubly nonnegative relaxation of the related copositive program
$\text{Feas}(\cdot)$	Feasible region of a given optimization problem
$\mathcal{E}(\cdot)$	Extreme points of a given set
$\text{Conv}(\cdot)$	Convex hull of a given set
$\text{Cone}(\cdot)$	Conic hull of a given set
$\text{cl}(\cdot)$	Closure of a given set
$\text{int}(\cdot)$	Interior of a given set

Chapter 1

INTRODUCTION

Copositive optimization (coined in [11]) is a special case of conic optimization, which is concerned with the optimization of a linear objective function over the convex cone of copositive or completely positive matrices subject to linear equality constraints. Therefore, it is a subfield of convex optimization.

In 2009, Burer [18] established that nonconvex quadratic programs with a mix of binary and continuous variables and linear constraints, hereinafter referred to as a *mixed binary quadratic program*, can be equivalently reformulated as a conic optimization problem over the cone of completely positive matrices. This is a remarkable result showing that a large class of nonconvex and NP-hard optimization problems can be reformulated as a convex optimization problem. Nevertheless, Burer's reformulation [18] of mixed binary quadratic programs does not change the complexity of the problem since the cone of completely positive matrices is computationally intractable. For this reason, various inner and outer approximation hierarchies, which approximate the intractable cone of completely positive matrices, have been proposed in the literature.

These approximation hierarchies are based on obtaining a series of tractable cones which yield increasingly better approximations of the intractable cone of completely positive matrices as the *level* of hierarchy increases. Therefore, for a mixed binary quadratic program (MBQP) with a minimization objective, one can obtain lower bounds on its optimal value by utilizing outer approximations of the completely positive cone in Burer's reformulation [18].

We remark that obtaining a lower bound on (MBQP) is, in general, nontrivial since the continuous relaxation of a given instance of (MBQP) obtained by relaxing the binary constraints remains a nonconvex and NP-hard problem in general. Therefore, outer approximations offer a good framework for finding lower bounds on the optimal value of (MBQP). Given a feasible solution of (MBQP), these lower bounds can be important in assessing the quality of the feasible solution. Moreover, good lower bounds can be helpful for quickly identifying near optimal solutions and can thus considerably improve the effectiveness of the solution methods such as branch-and-bound algorithms.

Motivated by these observations, we focus on the following optimization problems, all of which are special cases of (MBQP) and therefore can be equivalently formulated as copositive optimization problems:

- Mixed binary integer programs (MBP)
- 0-1 Knapsack problem (KP)
- Standard quadratic programs (StQP)

In this dissertation, we focus on the bounds arising from *outer* approximations of the copositive formulation of the aforementioned classes of optimization problems. We refer the reader to [91] for a unified analysis on the *inner* approximations of the completely positive formulation of mixed binary quadratic programs. In particular, we attempt to shed light on the following questions regarding the bounds obtained from outer approximations:

- *Comparison of bounds:* What is the quality of bounds arising from outer approximations compared to the bounds provided by the LP relaxations of (MBP) and (KP)?

- *Exactness:* Under what conditions do the bounds given by the outer approximations match the optimal value of the original problem, i.e., what are the sets of instances on which outer approximations are exact?

For (MBP) (resp. (KP)), we study the quality of lower (resp. upper) bounds arising from outer approximations in *comparison* with the linear programming (LP) relaxation of the related problem. We also investigate the extensions of our results to the more general case of (MBQP) with a quadratic objective function.

As for (StQP), inner and outer polyhedral approximations have already been extensively studied. Yıldırım [89] establishes tight error bounds on the gap between the upper and lower bounds arising from polyhedral approximations. In [84], Sağol and Yıldırım give a complete algebraic description of the instances of (StQP) on which lower and upper bounds arising from polyhedral approximations become exact at a finite level of the hierarchy. They also identify the structural properties of the instances of (StQP) for which the upper and lower bounds are exact only in the limit. Therefore, for (StQP), we will focus on the instances of (StQP) that admits an *exact* doubly nonnegative relaxation.

In brief, our main goal in this dissertation is to investigate the quality of bounds arising from the outer approximations of the completely positive formulation of the optimization problems given above.

In this chapter, we first provide a background and a brief literature review on copositive optimization in Section 1.1. We then present the motivation of this study in Section 1.2. Finally, contributions and the outline of this dissertation are provided in Section 1.3.

1.1 Background and Literature

In the world of optimization problems, there is a clear trade-off between generality and algorithmic efficiency, meaning that, the more general a problem becomes, the less efficient algorithms exist to solve it and vice versa. In this context, linear programming constitutes an example of extreme case, as there are very efficient algorithms for solving LP problems (e.g., the simplex method [21], and interior-point methods [44]). However, not every optimization problem can be formulated as LP, and in fact, LP corresponds to a rather specific class of optimization problems.

Convex optimization, on the other hand, is a much broader class of optimization problems, but it still enjoys a very rich duality theory similar to that of linear programming despite some complications as to the strong duality property. By the seminal work of Nesterov and Nemirovski [70], it has been shown that all convex optimization problems can be solved in polynomial-time as long as they admit efficiently computable self-concordant barrier functions.

Conic optimization is comprised of linear optimization problems over an affine subspace of a convex cone. In fact, all convex optimization problems can be reformulated as a conic optimization problem [71]. While still preserving the generality and all strengths of convex optimization mentioned above, interpretation of the dual problem in conic optimization is easier than that of a general convex optimization problem. Moreover, many nonconvex and combinatorial optimization problems can also be represented within the framework of conic optimization. Therefore, conic optimization occupies an important place in the world of mathematical optimization. Copositive optimization, being a special case of conic optimization, is therefore an attractive research area for many researchers, although the problems of this class are NP-hard in general.

The term "copositive" can be traced back to a report in 1952 by Motzkin [67]. Later in 1958, Hall [36] coined the completely positive matrices which originated in the study of inequality theory and quadratic forms. Since then copositivity and complete positivity have been studied by many researchers (for surveys, see [6] and [41]). However, introduction of these cones into optimization problems has emerged only in the last two decades.

Preisig's paper [80] in 1996 was one of the early studies that establishes a relation between the solution of a quadratic optimization problem and copositivity.

Quist et al. [81] proposed in 1998 that one can get a tighter version of the semidefinite programming (SDP) relaxations of the quadratic programs by utilizing the completely positive cone. Using the membership constraints of the copositive and completely positive cones in conic optimization firstly emerged in their study.

Bomze et al. [11] was the first to show that an NP-hard problem, namely standard quadratic programs, can be formulated as an equivalent copositive optimization problem. Their paper [11] is also where the term "copositive optimization" is coined. After their study, various nonconvex and combinatorial optimization problems have been shown to admit an equivalent copositive reformulation. In 2009, Burer [18] extended these results and showed that a rather larger class of optimization problems, namely mixed binary quadratic programs, can be formulated as an equivalent copositive program. The reader is referred to the surveys [9, 29] for further details in copositive optimization. Copositive reformulations do not change the complexity of the problem, but these studies have inspired many researchers to construct approximation frameworks and obtain bounds on the original problem.

Parrilo [73] was the first who constructed a sequence of convex cones satisfying

$$\mathcal{CP} \subseteq \ldots \subseteq \mathcal{Q}_1 \subseteq \mathcal{Q}_0 = \mathcal{DN} \quad \text{and} \quad \mathcal{CP} = \bigcap_{r\in\mathbb{N}} \mathcal{Q}_r.$$

Each of the convex cones $\mathcal{Q}_r$, $r \in \mathbb{N}$, can be represented by Linear Matrix Inequalites (LMIs). Therefore a conic optimization problem over $\mathcal{Q}_r$ is an SDP. There are also several polyhedral approximation hierarchies satisfying the similar relations to those of Parrilo's hieararchy. However, unlike Parrilo's approximations, problems arising from polyhedral approximations amounts to solving an LP problem. Detailed information on approximation hierarchies is provided in Chapter 2 (see also, e.g. [13, 17, 22, 24, 53, 54, 74, 89]).

Approximations proposed to the intractable cones $\mathcal{CP}$ and $\mathcal{COP}$ gave rise to another question: What is the quality of bounds arising from the outer approximations of the completely positive formulations of (MBQP)?

A unified analysis on the behavior of inner approximations of the completely positive formulation of (MBQP) has been done in [91]. Under the class of (MBQP), quality of bounds arising from inner and outer polyhedral approximations of (StQP) have been extensively studied [84, 89] as discussed in the previous section. Therefore, we study the doubly nonnegative relaxations of (StQP).

Our theoretical results contribute to the literature in the assessment of the quality of lower bounds arising from the outer approximatons of the copositive formulations of three different classes of optimization problems: (MBP), (KP) and (StQP).

1.2 Motivation

There is no efficient algorithm to solve general nonconvex optimization problems in general. Solution methods for this class of problems usually consist of dividing the problem into smaller subproblems, solving a relaxation of the subproblem in order to obtain lower bounds and employing some local search methods to obtain a feasible solution and hence an upper bound. For some classes of nonconvex optimization problems, straightforward relaxations of this class of problems even turn out to be NP-hard. The continuous relaxation of an instance of (MBQP) can be given as an example to this situation. It is easily verified that the continuous relaxation obtained by relaxing the binary constraints of (MBQP) is still nonconvex and NP-hard in general.

Therefore, obtaining bounds on the optimal values of these problems and investigating the tightness of these bounds is a valuable effort. Finding near-optimal solutions and good bounds can decrease the solution time by enabling solution methods to work more efficiently such as decreasing the number of nodes that will be evaluated in branch-and-bound type algorithms or shrinking the search area for heuristics.

Prior to Burer's result [18], various nonconvex and NP-hard optimization problems were known to admit a copositive reformulation [11, 78, 79]. Burer [18] established that copositive reformulation can be extended to a rather large class of optimization problems, namely, mixed binary quadratic programs. This makes it possible to study these nonconvex problems from the viewpoint of convex optimization. Although Burer's copositive reformulation is still NP-hard due to the intractable cone $\mathcal{CP}$, by employing a hierarchy of tractable approximations, it paves the way for obtaining bounds on the optimal value of the original problem in a reasonable time.

Motivated by this, we study the tractable cones that provide approximations to $\mathcal{CP}$. In particular, we focus on two specific outer approximations: a hierarchy of outer polyhedral approximations and the doubly nonnegative cone. When $\mathcal{CP}$ is approximated by a polyhedral cone, the resulting problem becomes an LP problem. This helps in our analysis as the structure of the LP problem is well-known and modern solvers can solve very large-scale LP problems. On the other hand, although the doubly nonnegative cone is non-polyhedral, when we use it to approximate $\mathcal{CP}$, the resulting problem can still be solved in polynomial-time (see, e.g. [31, 48, 90])

In this thesis, we focus on the copositive reformulations of three classes of optimization problems: mixed binary integer programs (MBP), 0-1 knapsack problem, and standard quadratic programs (StQP). Unless P = NP, there does not exist an efficient algorithm for solving these problems.

As for the reasons for studying these three problems, for (MBP), it is possible to make a comparison with its LP relaxation. To be more precise, we can compare the quality of lower bounds arising from outer approximations with that of the LP relaxation. This provides a nice edge in our analysis. The LP relaxation of the 0-1 knapsack problem, being a special case of (MBP), has a closed form solution. Exploiting that solution structure allows us to achieve even stronger results for the knapsack. Outer polyhedral approximations of (StQP) are already known to achieve good lower bounds and have been studied in [84, 89]. Therefore, we focus on the doubly nonnegative relaxation of (StQP).

In this dissertation, we attempt to shed light on the quality of outer approximations arising from the completely positive reformulations of certain nonconvex optimization problem classes discussed above. We hope that our results serve as a basis for studying the bounds for the general class of mixed binary quadratic programs in the future. Furthermore, our findings may lead to more refined outer approximations exploiting the strengths and avoiding the weaknesses of the outer approximations studied in this thesis.

1.3 Contributions and Outline

This dissertation mainly contributes to the following classes of optimization problems:

Mixed Binary Integer Programs

We define the sign preserving outer approximations, which is a more general definition that covers a large class of outer approximations of the copositive reformulation of mixed binary integer programs. Under the assumption that the feasible region of the original problem is nonempty, we show that outer approximations are unbounded if and only if the original problem is unbounded.

We compare the lower bounds arising from outer approximations with that of the LP relaxation of (MBP). Given an instance of (MBP), we show that lower bounds arising from sign preserving outer approximations are at least as good as the lower bound obtained from its LP relaxation. We also compare the feasible regions of outer approximations with that of the LP relaxation of (MBP). We give a characterization of the equality of these feasible regions. Note that this characterization is based on enumerating the extreme points of the feasible region of the LP relaxation. As such, it may not work in polynomial-time with respect to the problem size. Therefore, for outer approximations, we also give sufficient or necessary conditions that work in polynomial-time to compare the feasible regions.

We then attempt to extend our results to the mixed binary quadratic programs.

We provide characterizations for the unboundedness of (MBQP), the continuous relaxation of (MBQP), and characterizations (or sufficient conditions) for the unboundedness of outer approximations within our scope. We show that if continuous relaxation of (MBQP) is unbounded, then the outer polyhedral approximation at hierarchy level 0 must be unbounded as well. Furthermore, we provide illustrative examples for different possible cases.

As for the doubly nonnegative relaxations, we show by examples that there is no relationship with the continuous relaxation in terms of unboundedness. We next show that, in contrast with (MBP), lower bounds arising from the outer approximations of the completely positive formulation of (MBQP) are not comparable to the lower bound provided by the continuous relaxation, in general. However, we give a sufficient condition in Proposition 7, under which lower bounds arising from outer approximations are at least as good as the lower bound given by the continuous relaxation. We also present a sufficient condition under which outer approximations provide strictly better lower bounds than the lower bounds given by the continuous relaxation of (MBQP). We discuss the classes of optimization problems to which our results apply.

0-1 Knapsack Problem

We study two alternative completely positive formulations of the 0-1 knapsack problem. We compare the outer approximations arising from the formulations with the LP relaxation of (KP). We show that the upper bound given by the outer polyhedral approximations of each copositive formulation is equal to the upper bound given by the LP relaxation of (KP) until at least a certain level of the hierarchy. We argue that, at this level, the LP problem arising from these outer approximations has already exponentially many variables. For that reason, we conclude that outer polyhedral approximations perform poorly for the 0-1 knapsack problem and thus we do not recommend using them as an approximation framework for the 0-1 knapsack problem.

We also establish a sufficient condition that shows that, depending on the instance, the equality between the upper bounds given by outer polyhedral approximations and LP relaxation of (KP) can still persist in even at higher hierarchy levels. By that sufficient condition, we also give a closed formula about how much this level can rise.

As for the doubly nonnegative (DNN) relaxations, we show that they give strictly better bounds than the LP relaxation of (KP) if the LP relaxation has a non-integer unique optimal solution. We also provide an example illustrating that the uniqueness assumption cannot be relaxed in general.

Standard Quadratic Programs

For a given instance of (StQP), recognizing whether it admits an exact doubly nonnegative relaxation is important, because one can then solve the polynomial-time solvable DNN relaxation instead of solving the NP-hard original problem and still get the optimal value of the original problem.

In this study, we investigate the instances of (StQP) with an exact DNN relaxation. We give a complete algebraic characterization for the set of instances with an exact DNN relaxation ($\mathcal{Q}$). By relying on the characterization of $\mathcal{Q}$, we identified three subsets of $\mathcal{Q}$, all of which are convex cones with a polynomial-time membership oracle. None of the three sets is a subset of the other two sets as we show by examples in Section 5.5. We also show that there are still elements that belong $\mathcal{Q}$ and are not members of any of the three subsets. Therefore, the complexity of the membership problem in $\mathcal{Q}$ is still unknown.

The remainder of the dissertation is organized as follows: We discuss copositive and completely positive optimization in more detail in Chapter 2. We also introduce various approximation hierarchies constructed for the copositive and completely positive cones. Chapters 3, 4 and 5 focus on the outer approximations of the copositive formulations of mixed binary integer programs, 0-1 knapsack problem, and standard quadratic programs, respectively. Finally, in Chapter 6, we conclude the dissertation by a summary of our results and present some open questions.

The standard notation given in the nomenclature will be used throughout the thesis. Also, at the beginning of each chapter, additional notations specific to that chapter will be given if required.

Chapter 2

COPOSITIVE AND COMPLETELY POSITIVE OPTIMIZATION

Copositive and completely positive matrices have various applications, including control theory [42], block designs [37], economic modelling [33], a Markovian model of DNA evolution, complementarity problems, and maximin efficiency-robust tests (see [6] and the references therein). Recent applications also include clustering and data mining [26], and dynamical systems [5, 65].

Recently, copositive and completely positive matrices have received significant attention in the area of mathematical optimization since it has been proven that many combinatorial and nonconvex quadratic optimization problems admit a copositive reformulation. As all the other constraints are linear, this formulation transfers difficulty entirely into the conic constraint. This has created a completely different perspective on combinatorial and nonconvex quadratic optimization problems and has greatly increased the interest in copositive and completely positive optimization (see [9, 29] for surveys on copositive programming).

This chapter is organized as follows: First, basic definitions from convex analysis are provided. We define a set of convex cones including copositive and completely positive cones, which will be of high importance throughout this dissertation. We then introduce conic optimization and two special cases of conic optimization: copositive and completely positive optimization. We present Burer's completely positive formulation of mixed binary quadratic programs. We discuss outer approximations of the completely positive cone and the bounds arising from them. Finally, the scope of this thesis is presented.

2.1 Basics from Convex Analysis

In this section, we give some basic definitions from convex analysis. First we provide the definitions of a convex set and a convex combination, and then we give a fundamental theorem about convex cones.

Definition 1. *A set $\mathcal{C} \subseteq \mathbb{R}^n$ is called a convex set if for any $x \in \mathcal{C}$ and $y \in \mathcal{C}$, $\lambda x + (1-\lambda)y \in \mathcal{C}$ for all $\lambda \in [0,1]$.*

Definition 2. *Given $x^1, \ldots, x^k \in \mathbb{R}^n$ and $k \in \mathbb{N}$, a vector of the form*

$$x^0 = \lambda_1 x^1 + \ldots + \lambda_k x^k,$$

where $\lambda_i \in \mathbb{R}_+$, $i = 1, \ldots, k$ and $\sum_{i=1}^k \lambda_i = 1$, is called a convex combination.

Note that a set $\mathcal{C} \subseteq \mathbb{R}^n$ contains all convex combinations of its elements if and only if it is convex. We now give the definition of a cone.

Definition 3. *A set $\mathcal{K} \subseteq \mathbb{R}^n$ is called a cone if $\lambda x \in \mathcal{K}$ for all $x \in \mathcal{K}$ and for all $\lambda \geq 0$.*

We next provide the following theorem which shows that convex cones are closed under addition.

Theorem 1 ([82], Theorem 2.6)**.** *A cone $\mathcal{K} \subseteq \mathbb{R}^n$ is convex if and only if the following condition is satisfied:*

$$x \in \mathcal{K} \text{ and } y \in \mathcal{K} \implies x + y \in \mathcal{K}. \tag{2.1}$$

We now present the definitions of polyhedral, pointed and full-dimensional cones.

Definition 4. *A convex cone* $\mathcal{K} \subseteq \mathbb{R}^n$ *is a polyhedral cone, if it is the intersection of a finite number of half-spaces, i.e.,*

$$\mathcal{K} = \{x \in \mathbb{R}^n : Ax \geq 0\},$$

where $A \in \mathbb{R}^{m \times n}$.

Definition 5. *A cone* $\mathcal{K} \subseteq \mathbb{R}^n$ *is pointed if* $\mathcal{K} \cap (-\mathcal{K}) = \{0\}$.

Definition 6. *A cone* $\mathcal{K} \subseteq \mathbb{R}^n$ *is full-dimensional if it has a nonempty interior. As a result, the dimension of* $\mathcal{K}$ *is equal to* n.

We now introduce the definition of proper cone, which has all the properties given above.

Definition 7. *A cone* $\mathcal{K} \subseteq \mathbb{R}^n$ *is a proper cone, if it is convex, closed, pointed and full-dimensional.*

We will give the definition of dual cone, but first we need the following definition.

Definition 8. *An inner product space is a vector space* $\mathbb{V}$ *over* $\mathbb{R}$ *together with an inner product, i.e., with a map*

$$\langle \cdot, \cdot \rangle : \mathbb{V} \times \mathbb{V} \to \mathbb{R}$$

that satisfies the following three properties for all vectors $u, w, v \in \mathbb{V}$ *and all scalars* $\lambda \in \mathbb{R}$*:*

- *Conjugate symmetry:* $\langle u, w \rangle = \langle w, u \rangle$.
- *Bilinearity:* $\langle \lambda u, w \rangle = \lambda \langle u, w \rangle$ *and* $\langle u + w, v \rangle = \langle u, v \rangle + \langle w, v \rangle$.
- *Positive-definiteness:* $\langle u, u \rangle \geq 0$ *and* $\langle u, u \rangle = 0 \iff u = 0$.

Throughout this dissertation, the inner product in the n-dimensional Euclidean space is defined as $\langle u, v\rangle := u^T v = \sum_{i=1}^{n} u_i v_i$ and the inner product in the space of $m \times n$ matrices is defined as $\langle U, V\rangle := \text{trace}(U^T V) = \sum_{i=1}^{m}\sum_{j=1}^{n} U_{ij}V_{ij}$.

Definition 9. *For a set $\mathcal{C} \subseteq \mathbb{R}^n$, the dual cone with respect to the inner product $\langle\cdot,\cdot\rangle$ is given by*

$$\mathcal{C}^* := \{x \in \mathbb{R}^n : \langle x, y\rangle \geq 0 \textit{ for all } y \in \mathcal{C}\}$$

We have the following properties related to dual cones.

Proposition 1. *Let $\mathcal{K},\ \mathcal{K}_1,\ \mathcal{K}_2 \subseteq \mathbb{R}^n$ be cones. Then,*

(i) $\mathcal{K}^*$ *is always closed and convex.*

(ii) $\mathcal{K}_1 \subseteq \mathcal{K}_2$ *implies* $\mathcal{K}_2^* \subseteq \mathcal{K}_1^*$.

(iii) *If $\mathcal{K}$ has a nonempty interior, then $\mathcal{K}^*$ is pointed.*

(iv) *If $\text{cl}(K)$ is pointed, then $\mathcal{K}$ has a nonempty interior.*

(v) $K^{**} = \text{cl}(\text{Conv}(\mathcal{K}))$.

Suppose $\mathcal{K}$ is a proper cone. Then, by Proposition 1, $\mathcal{K}^*$ is also proper. Furthermore, since $\mathcal{K}$ is closed and convex, $\mathcal{K}^{**} = \mathcal{K}$.

Definition 10. *A set $\mathcal{C} \subseteq \mathbb{R}^n$ is called self-dual if $\mathcal{C} = \mathcal{C}^*$.*

Among the self-dual cones, nonnegative orthant, positive semidefinite cone and second order cone can be given. However, a cone does not have to be self-dual, e.g., copositive and completely positive cones.

Definition 11. *Given a set $\mathcal{C} \subseteq \mathbb{R}^n$, the convex hull of $\mathcal{C}$, denoted as* $\text{Conv}(\mathcal{C})$*, is the set of all convex combinations of the elements in $\mathcal{C}$, i.e.,*

$$\text{Conv}(\mathcal{C}) = \left\{ \sum_{i=1}^{k} \lambda_i x^i : x^i \in \mathcal{C},\ \lambda_i \geq 0,\ \sum_{i=1}^{k} \lambda_i = 1,\ k \in \mathbb{N} \right\},$$

which is also the smallest convex set that contains $\mathcal{C}$.

Definition 12. *Given a set $\mathcal{C} \subseteq \mathbb{R}^n$, the conic hull of $\mathcal{C}$, denoted as* $\text{Cone}(\mathcal{C})$*, is the set of all conic combinations of the elements in $\mathcal{C}$, i.e.,*

$$\text{Cone}(\mathcal{C}) = \left\{ \sum_{i=1}^{k} \lambda_i x^i : x^i \in \mathcal{C},\ \lambda_i \geq 0,\ k \in \mathbb{N} \right\},$$

which is also the smallest convex cone that contains $\mathcal{C}$.

2.2 Convex Cones

We first present the definitions of positive semidefinite, copositive and completely positive matrices and cones.

Definition 13. *A matrix $X \in \mathcal{S}^n$ is positive semidefinite if*

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

The cone of positive semidefinite matrices, henceforth referred to as the positive semidefinite cone, is denoted by

$$\mathcal{PSD} = \left\{ X \in \mathcal{S}^n : u^T X u \geq 0, \quad \forall u \in \mathbb{R}^n \right\}.$$

Note that we do not include dimension information in our cone notations; however, the dimension will always be clear from the context.

Definition 14. *A matrix $X \in \mathcal{S}^n$ is copositive if*

$$u^T X u \geq 0 \text{ for all } u \in \mathbb{R}^n_+.$$

The cone of copositive matrices, henceforth referred to as the copositive cone, is denoted by

$$\mathcal{COP} = \left\{ X \in \mathcal{S}^n : u^T X u \geq 0, \quad \forall u \in \mathbb{R}^n_+ \right\}.$$

Definition 15. *A matrix $X \in \mathcal{S}^n$ is completely positive if it can be decomposed as*

$$X = YY^T \textit{ for some } Y \in \mathbb{R}^{n \times k}_+. \tag{2.2}$$

Given a completely positive matrix $X \in \mathcal{S}^n$, the smallest $k \in \mathbb{N}$, for which the representation (2.2) is possible, is called the cp-rank of X. Finding the cp-rank of a given completely positive matrix still remains an open problem. To see some established bounds on the cp-rank, the reader is referred to [14, 15, 86, 87].

The cone of completely positive matrices, henceforth referred to as the completely positive cone, is denoted by

$$\mathcal{CP} = \left\{ X \in \mathcal{S}^n : X = \sum_{i=1}^{k} y^i (y^i)^T, \text{ for some } y^i \in \mathbb{R}^n_+, \ i = 1, \ldots, k \right\},$$

Note that copositive and completely positive cones are dual to each other, i.e., $(\mathcal{CP})^* = \mathcal{COP}$. Both cones are intractable cones, i.e., there are no known polynomial-time algorithms for checking the membership in $\mathcal{CP}$ and $\mathcal{COP}$. It has been proved that deciding where a given matrix is in $\mathcal{COP}$ is co-NP-complete [69]. As for $\mathcal{CP}$, the same complexity is anticipated, and it was established that checking the membership in $\mathcal{CP}$ is NP-hard [25, 69]. It is still an open question whether checking the membership in $\mathcal{CP}$ is also NP-complete. Interested reader is referred to [4] for the open questions in the theory of copositive and completely positive matrices.

We denote the cone of symmetric entrywise nonnegative matrices by $\mathcal{N}$ and refer to it as the nonnegative cone. $\mathcal{DN}$ denotes the intersection of positive semidefinite and nonnegative cones, and is called the doubly nonnegative cone, i.e., $\mathcal{DN} = \mathcal{PSD} \cap \mathcal{N}$. Lastly, we define the following cone

$$\mathcal{SPN} := \mathcal{PSD} + \mathcal{N} = (\mathcal{DN})^*.$$

Each of the cones $\mathcal{PSD}$, $\mathcal{COP}$, $\mathcal{CP}$, $\mathcal{N}$, $\mathcal{DN}$ and $\mathcal{SPN}$ is a proper cone and the following set of inclusion relations is satisfied:

$$\mathcal{CP} \subseteq \mathcal{DN} \subseteq \left\{ \begin{matrix} \mathcal{N} \\ \mathcal{PSD} \end{matrix} \right\} \subseteq \mathcal{SPN} \subseteq \mathcal{COP}.$$

We have $\mathcal{CP} = \mathcal{DN}$ and $\mathcal{SPN} = \mathcal{COP}$ if and only if $n \leq 4$ [23]. For the case $n = 5$, a well-known copositive matrix which does not belong to $\mathcal{SPN}$ is the Horn matrix [35], which can be given as

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix} \in \mathcal{COP} \setminus \mathcal{SPN}.$$

By utilizing the Horn matrix, the following matrix satisfies $\langle A, H \rangle < 0$

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 3 \end{bmatrix} \in \mathcal{DN} \setminus \mathcal{CP},$$

which is taken from [4].

2.3 Conic Optimization

A general formulation of a conic optimization problem can be given as

$$\begin{aligned} (P) \quad p^* := \min \quad & \langle c, x \rangle \\ \text{s.t.} \quad & \langle a_i, x \rangle = b_i, \quad i = 1, \ldots, m, \\ & x \in \mathcal{K}, \end{aligned}$$

where $x \in \mathbb{R}^n$ is the decision variable, $c \in \mathbb{R}^n$, $a_i \in \mathbb{R}^n$, $b_i \in \mathbb{R}$, $i = 1, \ldots, m$ are the problem parameters, and $\mathcal{K} \subseteq \mathbb{R}^n$ is a closed convex cone. Note that in (P), if the cone $\mathcal{K}$ is replaced by the nonnegative orthant ($\mathbb{R}^n_+$) and the Euclidean inner product is used, this gives rise to an LP problem. Therefore, linear programming is a special case of conic optimization. The associated dual problem of (P) is given by

$$\begin{aligned} (D) \quad d^* := \max \quad & b^T y \\ \text{s.t.} \quad & \sum_{i=1}^{m} y_i a_i + s = c, \\ & s \in \mathcal{K}^*, \end{aligned}$$

where $y \in \mathbb{R}^m$ and $s \in \mathbb{R}^n$ are the decision variables. The following lemma shows that *weak duality* always holds between primal and dual problems.

Lemma 1 (Weak Duality). *For all* $x \in \text{Feas}(P)$ *and* $(y, s) \in \text{Feas}(D)$*, we have*

$$\langle c, x \rangle \geq b^T y.$$

Therefore, $p^* \geq d^*$*.*

Proof. For all $x \in \text{Feas}(P)$ and $(y, s) \in \text{Feas}(D)$

$$\langle c, x \rangle - b^T y = \langle c, x \rangle - \sum_{i=1}^{m} \langle a_i, x \rangle y_i = \left\langle c - \sum_{i=1}^{m} y_i a_i, x \right\rangle = \langle s, x \rangle \geq 0,$$

since $x \in \mathcal{K}$, $s \in \mathcal{K}^*$ and by the Definition 9 of the dual cone. □

Lemma 1 shows that the objective value of any primal (resp. dual) feasible solution gives an upper (resp. lower) bound on the optimal value of the dual (resp. primal) problem. Given $x \in \text{Feas}(P)$ and $(y, s) \in \text{Feas}(D)$, the nonnegative value $\langle s, x \rangle = \langle c, x \rangle - b^T y$ is called the *duality gap*. Obviously, if the duality gap is zero, then x and (y, s) are optimal solutions of (P) and (D), respectively. It is well-known that the converse is also true in the case of linear programming, i.e., all pairs of primal-dual optimal solutions for an LP problem provides a zero duality gap (see, e.g. [85]). However, this is not necessarily true for conic optimization in general.

If the inequality $p^* \geq d^*$ implied by Lemma 1 is satisfied as equality, then such a situation is called the *strong duality*. Under regularity assumptions such as Slater's condition, it can be proven that strong duality is also satisfied between problems (P) and (D) (see, e.g., [88, Theorem 2.7] for a proof). Let relint$(\cdot)$ denote the relative interior [16]. Problem (P) satisfies Slater's condition if and only if it has a *strictly feasible solution*, i.e.,

$$\exists \hat{x} \text{ s.t. } \langle a_i, \hat{x} \rangle = b_i, \ i = 1, \ldots, m, \text{ and } \hat{x} \in \text{relint}(\mathcal{K}).$$

Linear programming is a significant subfield of the conic optimization since there exist efficient solution methods to solve LP problems both computationally and theoretically. For instance, the simplex method, developed by Dantzig [21] in 1947, was the first efficient method to solve LP problems in practice, although it does not work in polynomial-time in the worst case [50]. Later in 1979, Khachiyan [47] applied the ellipsoid method to derive the first polynomial-time algorithm for solving LP problems. Although it works better than the simplex method in theory, it remains slow in practice and is not competitive with simplex in general. Lastly, Karmarkar's algorithm [44], introduced in 1984, is another polynomial-time algorithm that falls in the class of interior-point methods and works very efficient in both theory and practice [58, 59, 66]. It also has better worst-time complexity than the ellipsoid method. Hence, linear programming has been an important class of optimization problems for more than six decades.

Another well-studied conic optimization problem is the semidefinite programming problem (SDP), which is defined over the positive semidefinite cone. After Karmarkar's interior-point method, Nesterov and Nemirovski [70] showed that this approach can be generalized to convex programming by employing self-concordant barrier functions. Their remarkable result implies that a conic optimization problem, e.g., SDP, can be solved in polynomial-time if the underlying convex cone admits a self-concordant barrier function that can be evaluated in polynomial-time. Therefore, interior-point methods are regarded as the most robust and efficient way for solving SDP problems.

LP and SDP are two of the most widely-studied problems in the optimization community. We are now in a position to introduce two special conic programs that constitute the theme of this dissertation, namely, copositive and completely positive programs.

2.4 Copositive Programs

A completely positive optimization problem is given by

$$
\begin{aligned}
\text{(CoP)} \quad \min \quad & \langle C, X \rangle \\
\text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \ldots, m, \\
& X \in \mathcal{CP},
\end{aligned}
$$

where $X \in \mathcal{S}^n$ is the decision variable, and $C \in \mathcal{S}^n$, $A_i \in \mathcal{S}^n$ and $b_i \in \mathbb{R}$, $i = 1 \ldots, m$, are the problem parameters. The dual problem of (CoP), called a copositive optimization problem, is given by

$$
\begin{aligned}
\text{(CoD)} \quad \max \quad & b^T y \\
\text{s.t.} \quad & \sum_{i=1}^{m} y_i A_i + S = C, \\
& S \in \mathcal{COP},
\end{aligned}
\tag{2.3}
$$

where $y \in \mathbb{R}^m$ and $S \in \mathcal{S}^n$ are the decision variables.

Despite involving different cones, both problems are often referred to simply as "copositive programs". Througout the remainder of this thesis, we also adopt this terminology.

Since (CoP) and (CoD) are both conic programs, the weak duality always holds between them and the strong duality holds under regularity conditions such as Slater's condition. Recall that the copositive and completely positive cones are convex, and all other constraints and the objective function are linear in both problems. Therefore (CoP) and (CoD) are convex optimization problems. However, as discussed before, both cones $\mathcal{CP}$ and $\mathcal{COP}$ are computationally intractable. Furthermore, several well-known NP-hard problems such as graph partitioning, maximum weighted clique, quadratic assignment, and standard quadratic optimization problems can be reformulated as an instance of (CoP). Therefore, as a consequence (CoP) and (CoD) are NP-hard problems in general [11, 79].

Copositive optimization has received considerable interest in the Operations Research community in recent years [9]. The main reason for this interest is due to an important discovery given in the following section.

2.5 Burer's Reformulation

In 2009, Burer [18] established that all mixed binary quadratic programs can be reformulated as a completely positive optimization problem (as an instance of (CoP)). Burer's this result also forms the basis of this thesis. By using the *lifting* procedure (see, e.g. [57]), he constructed a relaxation of the mixed binary quadratic programs but showed that it is, in fact, an equivalent reformulation. The problem he considered was

$$\begin{array}{lll} \text{(MBQP)} & \min & x^T Q x + c^T x \\ & \text{s.t.} & {a_i}^T x = b_i, \quad i = 1, \dots, m, \\ & & x \geq 0, \\ & & x_j \in \{0, 1\}, \quad j \in B, \end{array}$$

where $x \in \mathbb{R}^n$ is the decision variable; $Q \in \mathcal{S}^n$, $a_i \in \mathbb{R}^n$, $b \in \mathbb{R}^m$ and $B \subseteq \{1, \dots, n\}$ are the problem parameters. (MBQP) encompasses a rather large class of NP-hard problems, e.g., all mixed binary integer programs, all nonconvex (continuous) quadratic programs, and specific problems such as the quadratic assignment problem. Linear portion of Feas(MBQP) is given by

$$L := \{x \in \mathbb{R}^n : a_i^T x = b_i, \quad i = 1, \ldots, m, \ x \geq 0\}.$$

Without loss of generality, Burer [18] makes the following assumption, referred to as the *key assumption*:

$$x \in L \implies 0 \leq x_j \leq 1, \quad j \in B. \tag{2.4}$$

Note that if the key assumption does not hold, then it can always be ensured by augmenting (MBQP) with the constraints $x_j + s_j = 1$ and $s_j \geq 0$, $j \in B$. Under the key assumption (2.4), Burer [18] showed that (MBQP) can be equivalently reformulated as the following instance of (CoP):

$$\begin{array}{lll} \text{(MBQP-CP)} & \min & \langle Q, X \rangle + c^T x \\ & \text{s.t.} & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\ & & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\ & & x_j = X_{jj}, \quad j \in B, \\ & & \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{CP}, \end{array}$$

where $x \in \mathbb{R}^n$ and $X \in \mathcal{S}^n$ are the decision variables. Burer's main result in [18] is the following:

Theorem 2 ([18], Theorem 2.6)**.** (MBQP) *and* (MBQP-CP) *have the same optimal value. Furthermore, if* (x^*, X^*) *is an optimal solution for* (MBQP-CP)*, then* x^* *is in the convex hull of optimal solutions for* (MBQP)*.*

By this result, it has been shown that a large class of mixed binary quadratic optimization problems can be reformulated as a completely positive optimization problem. Therefore, (CoP) is a computationally intractable problem in general. Since the objective function and all the other constraints are linear, all the complexity is absorbed by the membership constraint of the cone $\mathcal{CP}$. In [12], Bomze and Jarre interpret Burer's result from a topological perspective. They also discuss why the feasibility of the copositive formulation implies the feasibility of the original mixed binary quadratic program. We refer the reader to [12, 18] for further details. This conic reformulation of Burer [18] paved the way for the recent studies in the field of copositive optimization [10, 12, 27, 54, 84, 89].

2.6 Outer Approximations

In this thesis, we focus on the outer approximations of the completely positive cone since a comprehensive analysis on the inner approximations of copositive formulations of mixed binary quadratic programs has already been done in [91]. Therefore, inner approximations will be out of the scope of this dissertation. However, the interested reader is referred to see [13, 89] for different works on the inner polyhedral approximations and [24, 53, 54] for those on the inner non-polyhedral approximations of the cone $\mathcal{CP}$.

Both $\mathcal{CP}$ and $\mathcal{COP}$ are intractable cones. Therefore, many studies in the literature have proposed various tractable approximation hierarchies for these cones. Most of these hierarchies are constructed based on the fact that a matrix $M \in \mathcal{S}^n$ is copositive if and only if the polynomial

$$P_M(x) := \sum_{i=1}^{n} \sum_{j=1}^{n} M_{ij} x_i^2 x_j^2 \tag{2.5}$$

is nonnegative for all $x \in \mathbb{R}^n$.

We begin with the formal definition of an *outer approximation hierarchy.*

Definition 16. *Given a closed convex cone $\mathcal{K} \subseteq \mathcal{S}^n$, a sequence of cones $\mathcal{C}_r \subseteq \mathcal{S}^n$, $r \in \mathbb{N}$, is called an outer approximation hierarchy if it satisfies the following relations:*

$$\mathcal{C}_0 \supseteq \mathcal{C}_1 \supseteq \ldots \supseteq \mathcal{K} \quad \textit{and} \quad \bigcap_{r \in \mathbb{N}} \mathcal{C}_r = \mathcal{K}.$$

By the properties of dual cones given in Proposition 1, this hierarchy can be converted into a hierarchy of the dual cone as follows:

$$\mathcal{C}_0^* \subseteq \mathcal{C}_1^* \subseteq \ldots \subseteq \mathcal{K}^* \quad \text{and} \quad \text{cl}\left(\bigcup_{r\in\mathbb{N}} \mathcal{C}_r^*\right) = \mathcal{K}^*.$$

Therefore, approximation hierarchies devised for the copositive cone can also be converted into an approximation hierarchy for the completely positive cone and vice versa.

We now introduce outer approximation hierarchies that are built to approximate the completely positive cone from outside. We start with a hierarchy of inner polyhedral approximations to the copositive cone introduced by de Klerk and Pasechnik [22] by exploiting the sufficient conditions for matrix copositivity. By duality, this results in a hierarchy of outer polyhedral approximations to the cone $\mathcal{CP}$. This section is concluded with a review of non-polyhedral approximation hierarchies.

2.6.1 Polyhedral Approximations

By duality, outer approximations of the cone $\mathcal{CP}$ can be derived from the inner approximations of the cone $\mathcal{COP}$. In the same manner, inner approximations of $\mathcal{COP}$ obtained by de Klerk and Pasechnik [22] yield outer approximations to $\mathcal{CP}$.

Let us define the following polynomial of degree $2(r+2)$:

$$P_M^r(x) := P_M(x)\left(\sum_{i=1}^{n} x_i^2\right)^r, \quad r \in \mathbb{N}, \tag{2.6}$$

where $P_M(x)$ is defined in (2.5). Recall that $M \in \mathcal{COP}$ if and only if $P_M(x) \geq 0$ for all $x \in \mathbb{R}^n$. Observe that nonnegativity of $P_M(x)$ is already guaranteed if $P_M^r(x) \geq 0$, $r \in \mathbb{N}$, for all $x \in \mathbb{R}^n$. By using the fact that $P_M^r(x)$ is nonnegative if all its coefficients are nonnegative, de Klerk and Pasechnik [22] defined the following sequence of cones

$$(\mathcal{O}_r)^* := \left\{M \in \mathcal{S}^n : P_M^r(x) \text{ has nonnegative coefficients}\right\}, \; r \in \mathbb{N},$$

and established that

$$\mathcal{N} = (\mathcal{O}_0)^* \subseteq (\mathcal{O}_1)^* \subseteq \ldots \subseteq \mathcal{COP} \quad \text{and} \quad \mathrm{cl}\left(\bigcup_{r\in\mathbb{N}} (\mathcal{O}_r)^*\right) = \mathcal{COP}. \tag{2.7}$$

Now, let us define

$$\Theta(n,r) := \left\{ z \in \mathbb{N}^n : \sum_{i=1}^{n} z_i = r+2 \right\}, \quad r \in \mathbb{N}. \tag{2.8}$$

de Klerk and Pasechnik [22] also showed that $(\mathcal{O}_r)^*$ can be rewritten as

$$(\mathcal{O}_r)^* = \{X \in \mathcal{S}^n : \langle zz^T - \mathrm{Diag}(z), X\rangle \geq 0 \text{ for all } z \in \Theta(n,r)\}, \quad r \in \mathbb{N}. \tag{2.9}$$

Therefore, $\mathcal{O}_r$ (the dual of $(\mathcal{O}_r)^*$) can be given as

$$\mathcal{O}_r = \left\{ \sum_{z\in\Theta(n,r)} \lambda_z \left(zz^T - \mathrm{Diag}(z)\right) : \lambda_z \geq 0 \text{ for all } z \in \Theta(n,r) \right\}, \quad r \in \mathbb{N}. \tag{2.10}$$

By duality, this implies

$$\mathcal{CP} \subseteq \ldots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0 = \mathcal{N} \quad \text{and} \quad \mathcal{CP} = \bigcap_{r\in\mathbb{N}} \mathcal{O}_r. \tag{2.11}$$

Therefore, this sequence of cones constitutes an outer approximation hierarchy to the completely positive cone. As $r \in \mathbb{N}$ increases, we get increasingly better approximations of $\mathcal{CP}$, and in the limit they converge to $\mathcal{CP}$.

It is easy to check that

$$|\Theta(n,r)| = \binom{n+r+1}{r+2} = O(n^{r+2}), \quad r \in \mathbb{N}. \tag{2.12}$$

By (2.12), $\mathcal{O}_r$ has a finite number of extreme rays and thus is polyhedral for each $r \in \mathbb{N}$. Since each cone $\mathcal{O}_r$ is polyhedral, a linear optimization problem over these cones is equivalent to an LP problem. However, by (2.12), it is important to note that as r increases the number of variables in the related LP problem grows exponentially with $\mathcal{O}(n^{r+2})$.

Bundfuss and Dür [17] also proposed outer approximation hierarchies for the copositive cone. Since they are adaptive and refined with respect to the objective function, their behaviour change according to the problem instance. Therefore, they are more algorithmic implementation-oriented and not appropraite for our analysis. As a result, we investigate the outer polyhedral approximation hierarchy proposed by de Klerk and Pasechnik [22].

We now discuss several hierarchies of outer non-polyhedral approximations to the completely positve cone.

2.6.2 Non-Polyhedral Approximations

Parrilo [73] was the first who employed an approximation approach for the copositive cone by using a hierarchy of tractable convex cones in his thesis. He basically exploited the fact that any polynomial that can be decomposed as a sum-of-squares (sos) is necessarily nonnegative.

Consider the polynomial $P^r_M(x)$ given in (2.5). Parrilo [73] defined the following sequence of cones:

$$(\mathcal{Q}_r)^* := \left\{ M \in \mathcal{S}^n : P^r_M(x) \text{ has an sos decomposition} \right\}, \; r \in \mathbb{N}.$$

He then showed that these cones satisfy the following relationship:

$$\mathcal{SPN} = (\mathcal{Q}_0)^* \subseteq (\mathcal{Q}_1)^* \subseteq \ldots \subseteq \mathcal{COP} \quad \text{and} \quad \text{cl}\left(\bigcup_{r \in \mathbb{N}} (\mathcal{Q}_r)^* \right) = \mathcal{COP}.$$

By duality, this implies

$$\mathcal{CP} \subseteq \ldots \subseteq \mathcal{Q}_1 \subseteq \mathcal{Q}_0 = \mathcal{DN} \quad \text{and} \quad \mathcal{CP} = \bigcap_{r \in \mathbb{N}} \mathcal{Q}_r.$$

Each of the convex cones $\mathcal{Q}_r$ can be represented by Linear Matrix Inequalites (LMIs). Therefore a linear optimization problem over these cones turns out to be a semidefinite programming (SDP) problem. However, as the level of hierarchy increases, instance size of the corresponding SDP problem grows exponentially.

Exploiting a weaker sufficient condition than that of Parrilo, in 2007, Pena et al. [74] constructed another hierarchy of convex cones satisfying $\mathcal{CP} \subseteq \ldots \subseteq \mathcal{K}_1 \subseteq \mathcal{K}_0 = \mathcal{DN}$. They also showed that $\mathcal{Q}_r \subseteq \mathcal{K}_r \subseteq \mathcal{O}_r$, where $\mathcal{O}_r$ is defined in (2.10), and $\mathcal{K}_r = \mathcal{Q}_r$ for $r = 0, 1$. Since each $\mathcal{K}_r$ can be represented by LMIs, a linear optimization problem over these cones is equivalent to an SDP problem. At levels higher than zero, both Parrilo's and Pena et al.'s hierarchies become inappropriate for a theoretical analysis due to their complicated structures. Therefore, among the non-polyhedral outer approximations we will only evaluate the cone $\mathcal{DN} = \mathcal{K}_0 = \mathcal{Q}_0$.

We also point out that in literature there exist some other approximation hierarchies to the copositive and completely positive cones. For further details, the reader is referred to [2, 27, 28].

2.7 Lower Bounds

By employing outer approximation hierarchies, one can approximate an intractable conic optimization problem by a sequence of tractable optimization problems. Recall that a completely positive program (CoP) is given by

$$\begin{aligned} \nu := \quad \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \ldots, m, \\ & X \in \mathcal{CP}, \end{aligned}$$

where $X \in \mathcal{S}^n$ is the decision variable, and $C \in \mathcal{S}^n$, $A_i \in \mathcal{S}^n$, and $b_i \in \mathbb{R}$, $i = 1 \ldots, m$ are the problem parameters. Since this problem is computationally intractable, we use the outer approximation hierarchies to obtain the lower bounds on the optimal value ν. More precisely, we replace the intractable cone $\mathcal{CP}$ by a sequence of increasingly better tractable outer approximations. By doing that, one can obtain increasingly tighter lower bounds on ν as the level of hierarchy increases. If we replace the conic constraint $X \in \mathcal{CP}$ by $X \in \mathcal{O}_r$, where $\mathcal{O}_r$, $r \in \mathbb{N}$, is defined as in (2.10), then we get the following problems:

$$\begin{aligned} \ell_r := \quad \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \ldots, m, \\ & X \in \mathcal{O}_r, \end{aligned} \tag{2.13}$$

where $r \in \mathbb{N}$. Recall that problems obtained by outer polyhedral approximations is equivalent to linear programming problems. However, the number of variables in the related LP problem grows exponentially. Therefore, as r increases, the corresponding LP problem quickly reach beyond today's computational capabilities. Hence, it is crucial to obtain tight bounds at low levels of hierarchy.

Note that since (CoP) is a minimization problem, ℓ_r, $r \in \mathbb{N}$, constitutes a lower bound on the optimal value. By (2.11), we also have

$$\ell_0 \leq \ell_1 \leq \ldots \leq \nu.$$

In [89, Theorem 3.1], Yıldırım states that if both problems (COP) and (CoD) (defined in (2.3)) have strictly feasible solutions, then bounds arising from his inner approximation hierarchy and de Klerk and Pasechnik's [22] outer approximation hierarchy both converge to ν in the limit. However, this assumption can be relaxed when only outer approximations due to de Klerk and Pasechnik [22] are considered. Therefore, we establish the following result which can also be derived from the proof of [89, Theorem 3.1].

Proposition 2. *If* (CoD) *has a strictly feasible solution and its set of optimal solutions is nonempty, then*

$$\lim_{r \to \infty} \ell_r = \nu.$$

Proof. Consider the problem (2.13). By linear programming duality, its dual is given by

$$\ell_r = \max \left\{ b^T y : \sum_{i=1}^{m} y_i A_i + S = C, \ S \in (\mathcal{O}_r)^* \right\}, \quad r \in \mathbb{N}, \tag{2.14}$$

where $(\mathcal{O}_r)^*$ is defined in (2.9). Let $(\hat{y}, \hat{S}) \in \mathbb{R}^m \times \mathcal{S}^n$ be a strictly feasible solution of (CoD). By (2.7), there exists $r_0 \in \mathbb{N}$ such that $\hat{S} \in (\mathcal{O}_r)^*$ for all $r \geq r_0$. This also implies $\hat{S}$ is a feasible solution of (2.14) for all $r \geq r_0$. Therefore,

$$b^T \hat{y} \leq \ell_r \leq \nu$$

holds for all $r \geq r_0$. Since the optimal solution of (CoD) is attainable, let (y^*, S^*) be an optimal solution of it. Let us also define $(y_\lambda, S_\lambda) := \lambda(y^*, S^*) + (1-\lambda)(\hat{y}, \hat{S})$. Observe that (y_λ, S_λ) is also a strictly feasible solution of (CoD) for all $\lambda \in (0,1)$. Therefore, by (2.7), for any $\lambda \in (0,1)$, there exists $r_\lambda \in \mathbb{N}$ such that (y_λ, s_λ) is a feasible solution of (2.14) for all $r \geq r_\lambda$. This implies that

$$b^T y_\lambda = \lambda b^T y^* + (1-\lambda) b^T \hat{y} \leq \ell_r \leq \nu = b^T y^*$$

holds for all $r \geq r_\lambda$. Therefore, as λ goes to 1 we have $\lim_{r \to \infty} \ell_r = \nu$. □

This proposition states that as long as (CoD) has a strictly feasible solution and an attainable optimal solution, the seqence of lower bounds obtained from (2.13) converge to the optimal value of (CoP).

In addition to the hierarchy of the outer polyhedral approximations proposed by de Klerk and Pasechnik [22], we will also analyze the *doubly nonnegative relaxations* arising from the doubly nonnegative cone, which corresponds to the first cone in the hierarchies of non-polyhedral approximations proposed by Parrilo [73] and Pena et al. [74].

Replacing the conic constraint $X \in \mathcal{CP}$ by $X \in \mathcal{DN}$, we obtain a doubly nonnegative relaxation of (CoP) as follows:

$$\begin{aligned} \ell_{DN} := \quad \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \ldots, m, \\ & X \in \mathcal{DN}, \end{aligned}$$

The resulting problem is not an LP problem, since the doubly nonnegative cone is non-polyhedral. However, it corresponds to a semidefinite programming problem and thus is still computationally tractable.

2.8 Our Scope

Optimization consists of finding a minimum or maximum value of an objective function subject to a set of constraints. There are various necessary or sufficient optimality conditions that have been proposed for optimization problems in the literature. The reader is referred to the books by Horst et al. [39, 40] for the related topic. However, for some optimization problems, obtaining a globally optimal solution in a reasonable time is not possible. Therefore, by employing various approximation techniques, obtaining tight bounds on the optimal value of such problems is a valuable pursuit for many researchers.

In this dissertation, we consider three specific problem classes related to nonconvex optimization: mixed binary integer programs, 0-1 knapsack problem and standard quadratic programs. Note that all these problems are NP-hard in general, and they are special cases of mixed binary quadratic programs. Nonconvexitiy of first two problems is due to their discrete structures, whereas that of standard quadratic programs is due to the quadratic objective function.

Mixed binary integer programs consist of a large class of optimization problems, including the 0-1 knapsack problem. The 0-1 knapsack problem appears in many real-world applications such as stock cutting, capital budgeting, portfolio selection, and asset-backed securitization problems (see [46] and the references therein). Although it is a special case of mixed binary integer programs, we can get stronger results for it since the optimal solution of its LP relaxation has a special structure. Therefore, we devote an entirely separate chapter to the 0-1 knapsack problem.

Standard quadratic programs have also many application areas, e.g., portfolio optimization [61], population genetics [49], evolutionary game theory [8] and maximum (weighted) clique problem [32, 68]. Therefore, we focus on these problem classes in this thesis.

We also attempt to extend our results to the mixed binary quadratic programs.

Burer's copositive reformulation opens up a new field of research for general non-convex linear or quadratic optimization problems. Therefore, we study copositive formulations of (MBP), (KP) and (StQP). Since these conic programs are still computationally intractable due to the intractability of the underlying cones, we focus on the outer approximations of them. We choose the hierarchy of outer polyhedral approximations proposed by de Klerk and Pasechnik [22] and the doubly nonnegative cone, which is the first cone in the hierarchies due to Parrilo [73] and Pena et al. [74].

Recall that replacing the conic constraint $X \in \mathcal{CP}$ by $X \in \mathcal{O}_r$, $r \in \mathbb{N}$, generates an LP problem, whereas replacing it by $X \in \mathcal{DN}$ generates an SDP problem. Therefore, polyhedral approximation hierarchies are relatively easier to analyze due to their simpler structures. However, we also obtain promising results from our analysis for doubly nonnegative relaxations.

In this dissertation, for the given problem classes and outer approximations we seek answers to the following questions:

- What is the quality of bounds arising from outer approximations compared to the bounds provided by the LP relaxations of (MBP) and (KP)?

- Under what conditions do the bounds given by the outer approximations match the optimal of the original problem, i.e., when do outer approximations become exact?

Our research concentrates on the comparison of bounds for (MBP) and (KP) problems in Chapter 3 and Chapter 4, respectively. For (StQP) problems, we consider the exactness of their doubly nonnegative relaxations in Chapter 5.

Chapter 3

OUTER APPROXIMATIONS OF MIXED BINARY INTEGER PROGRAMS

3.1 Introduction

We consider *mixed binary integer programs* (MBP). (MBP) can be given as

$$
\begin{aligned}
\text{(MBP)} \quad \nu := \quad \min \quad & c^T x \\
\text{s.t.} \quad & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\
& x \geq 0, \\
& x_j \in \{0, 1\}, \quad j \in B,
\end{aligned}
\tag{3.1}
$$

where $x \in \mathbb{R}^n$ is the decision variable; $a_i \in \mathbb{R}^n$, $b \in \mathbb{R}^m$ and $B \subseteq \{1, \ldots, n\}$ are problem parameters. Throughout this chapter, without loss of generality, we assume that Burer's *key assumption* [18] holds. Under that assumption, (MBP) can be equivalently formulated as

$$
\begin{aligned}
\text{(MBP-CP)} \quad \nu := \quad \min \quad & c^T x \\
\text{s.t.} \quad & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\
& {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\
& x_j = X_{jj}, \quad j \in B, \\
& \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{CP},
\end{aligned}
\tag{3.2}
$$

where $x \in \mathbb{R}^n$ and $X \in \mathcal{S}^n$ are decision variables. Both (MBP) and (MBP-CP) are NP-hard problems. Although (MBP-CP) is a convex optimization problem defined over the completely positive cone, the difficulty here is transferred into the conic constraint. In fact, for a given matrix $X \in \mathcal{S}^n$, deciding whether $X \in \mathcal{CP}$ is even NP-hard [25, 69]. Therefore, $\mathcal{CP}$ is intractable. Suppose, we replaced the intractable $\mathcal{CP}$ in (MBP-CP) by a tractable convex cone $\mathcal{K} \supseteq \mathcal{CP}$. Then, the new problem constitutes an outer approximation of (MBP-CP) and gives a lower bound on ν since (MBP-CP) is a minimization problem.

In this chapter, we aim to evaluate the feasible regions and optimal values of the various relaxations obtained from replacing $\mathcal{CP}$ in (MBP-CP) by certain outer approximations. In comparison with the relaxations of (MBP-CP) arising from outer approximations, we will also analyze the linear programming (LP) relaxation of (MBP), which is given by

$$\begin{array}{llll} \text{Rel(MBP)} & \ell_{LP} := & \min & c^T x \\ & & \text{s.t.} & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\ & & & x \geq 0. \end{array} \tag{3.3}$$

Note that we do not need the constraints $x_j \leq 1$, $j \in B$, since they are already implied by Burer's key assumption [18]. Since (MBP) is a minimization problem, optimal value of Rel(MBP) constitutes a lower bound on the optimal value of (MBP), i.e., $\ell_{LP} \leq \nu$.

This chapter is organized as follows: We will define our notation in Section 3.1.1. In Section 3.2, we will give a definition for *sign preserving outer approximations* (SPR). Given an instance of (MBP), we will compare the optimal values and feasible regions of (SPR) and Rel(MBP). In a similar manner, we will compare the relaxations arising from outer polyhedral approximations and Rel(MBP) in Section 3.3. Section 3.4 is devoted to the comparison of the doubly nonnegative relaxation of (MBP-CP) and Rel(MBP). We define *mixed binary quadratic program* (MBQP) in Section 3.5 and investigate the extensions of our results to (MBQP). We conclude the chapter in Section 3.6 by discussing the implication of our results.

3.1.1 Notation

e will denote the vector of all ones of appropriate dimension and $E = ee^T$ will denote the matrix of all ones. e_i will denote the standard unit vector whose i^{th} element is equal to 1 and all others are equal to 0. If A is an $n \times n$ matrix and $\alpha, \beta \subseteq \{1, \ldots, n\}$, then $A[\alpha|\beta]$ is the *submatrix* lying in the rows α and columns β. For brevity, the *principal submatrix* $A[\alpha|\alpha]$ will be denoted by $A[\alpha]$. Also for a vector $x \in \mathbb{R}^n$, $x[\alpha]$ will be the *subvector* of length $|\alpha|$ which consists of the elements of x indexed by α. Diag($\cdot$) returns a square diagonal matrix which consists of the entries of a given vector on the main diagonal.

Feas($\cdot$) will denote the feasible region of a given problem. Set of extreme points of a given set will be denoted by $\mathcal{E}(\cdot)$. Conv($\cdot$) will denote the convex hull of a given set. Given two matrices $X,\ Y \in \mathbb{R}^{m\times n}$, $\langle X, Y\rangle$ will denote the trace inner product, i.e.,

$$\langle X, Y\rangle = \sum_{i=1}^{m}\sum_{j=1}^{n} X_{ij}Y_{ij}.$$

3.2 A General Case: Sign Preserving Outer Approximations

In this section, we present a more general definition of outer approximation for (MBP-CP). We compare this outer approximation with Rel(KP) in terms of their feasible regions and the lower bounds they provide. Note that the results established here will also apply to the following sections and will serve as preliminary for our main results.

Suppose $\mathcal{K}$ is a closed convex cone such that $\mathcal{K} \supseteq \mathcal{CP}$. Recall that $\mathcal{K}$ constitutes an outer approximation for $\mathcal{CP}$. Replacing $\mathcal{CP}$ by $\mathcal{K}$ in the conic constraint, we get a relaxation of (MBP-CP). Now, we define the following convex optimization problem:

$$
\begin{aligned}
\text{(SPR)} \quad \ell_{sp} := \quad \min \quad & c^T x \\
\text{s.t.} \quad & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\
& {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\
& x_j = X_{jj}, \quad j \in B, \\
& \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{K},
\end{aligned} \tag{3.4}
$$

where $\mathcal{K} \supseteq \mathcal{CP}$. (SPR) will be referred to as the *sign preserving outer approximation* of (MBP-CP). We make following assumption regarding the cone $\mathcal{K} \supseteq \mathcal{CP}$:

$$
\begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{K} \implies x \geq 0. \tag{3.5}
$$

Note that if this assumption does not hold, then without loss of generality, nonnegativity of x can always be achieved by adding the constraint $x \geq 0$ to (SPR).

Since (SPR) is a relaxation of (MBP-CP), it follows that $\ell_{sp} \leq \nu$. We define the following set:

$$
F_{sp} := \{x \in \mathbb{R}^n : (x, X) \in \text{Feas(SPR)}\}. \tag{3.6}
$$

F_{sp} is basically the projection of the feasible region of (SPR) onto $\mathbb{R}^n$. Arising from the projection of a convex feasible region onto $\mathbb{R}^n$, F_{sp} is also convex. By (3.6), since the objective function of (SPR) is only dependent on $x \in \mathbb{R}^n$, as an immediate result, observe that (SPR) is equivalent to the following problem:

$$
\ell_{sp} = \min\{c^T x : x \in F_{sp}\}. \tag{3.7}
$$

This simple observation will help us while establishing our results.

3.2.1 Comparison of the Feasible Regions and Lower Bounds

In this section, we aim to compare the lower bounds given by (SPR) and Rel(MBP). Note that ℓ_{LP} can be given as follows:

$$\ell_{LP} = \min\{c^T x : x \in \text{Feas}(\text{Rel}(\text{MBP}))\}. \tag{3.8}$$

First, we give the following proposition which establishes a characterization for the unboundedness of the problems under consideration.

Proposition 3. *Suppose* Feas(MBP) *is nonempty. Following statements are equivalent:*

(i) (MBP) *is unbounded, i.e.,* $\nu = -\infty$.

(ii) Rel(MBP) *is unbounded, i.e.,* $\ell_{LP} = -\infty$.

(iii) (SPR) *is unbounded i.e.,* $\ell_{sp} = -\infty$.

(iv) There exists $d \in \mathbb{R}^n_+$ *such that* $c^T d < 0$, $a_i{}^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

Proof. It is easy to confirm that (MBP) and Rel(MBP) are bounded if and only if item (iv) holds. Now we will show $(iii) \iff (iv)$. $(iv) \implies (iii)$ follows from $(i) \implies (iii)$, since (SPR) is a relaxation of (MBP). Conversely, suppose (SPR) is unbounded. Since F_{sp} is a convex set, from (3.7), there exists $d \in \mathbb{R}^n$ such that $c^T d < 0$ and due to sign restriction of x, $d \geq 0$. Since $a_i{}^T x = b_i$ implies $x_j \leq 1$ for all $j \in B$, $d[B] = 0$ follows. This completes the proof. □

Proposition 3 is important in terms of showing that unless (MBP) is unbounded, (SPR) and Rel(MBP) always give finite lower bounds. Now, we will establish a relation between ℓ_{LP} and ℓ_{sp}. Next lemma establishes a relation between F_{sp} and Feas(Rel(MBP)), which also enables us to compare ℓ_{sp} and ℓ_{LP}.

Lemma 2. $F_{sp} \subseteq \text{Feas}(\text{Rel}(\text{MBP}))$*. As a result,* $\ell_{sp} \geq \ell_{LP}$*.*

Proof. Observe that together with the assumption (3.5) all the constraints of Rel(MBP) are implied by the constraints of (SPR). Therefore, we conclude the given inclusion. From (3.7) and (3.8), $\ell_{sp} \geq \ell_{LP}$ directly follows. □

This is a promising result, since Lemma 2 clearly establishes that the lower bounds given by sign preserving outer approximations of (MBP-CP) are at least as good as the lower bound given by Rel(MBP).

Given $x \in \text{Feas}(\text{Rel}(\text{MBP}))$, in the next lemma, we establish a characterization to determine if $x \in F_{sp}$ or not. This is a simple characterization, which directly follows from the formulation of (SPR), but later on we will use this lemma to produce more useful results.

Lemma 3. *Let* $\mathcal{K} \supseteq \mathcal{CP}$ *be the cone in the formulation of* (SPR)*. Let* $\hat{x}$ *be in the feasible region of* Rel(MBP)*.* $\hat{x} \in F_{sp}$ *if and only if the following problem is feasible:*

$$
\begin{array}{lll}
(P_{\hat{x}}) & \min & 0 \\
& \text{s.t.} & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\
& & X_{jj} = \hat{x}_j, \quad j \in B, \\
& & \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} \in \mathcal{K}.
\end{array}
$$

Proof. This result is easily derived by the formulation of (SPR). □

By Lemma 3, it follows that $F_{sp} = \text{Feas}(\text{Rel}(\text{MBP}))$ holds if and only if (P_x) is feasible for all $x \in \text{Feas}(\text{Rel}(\text{MBP}))$. This does not say much to us since Feas(Rel(MBP)) will highly likely have infinitely many points. However, suppose Feas(Rel(MBP)) is bounded. Observe that $F_{sp} \subseteq \text{Feas}(\text{Rel}(\text{MBP}))$, F_{sp} is a convex set and Feas(Rel(MBP)) is a polyhedron. Therefore, to confirm that $F_{sp} = \text{Feas}(\text{Rel}(\text{MBP}))$, it would be sufficient to solve (P_x) only for all $x \in \mathcal{E}(\text{Feas}(\text{Rel}(\text{MBP})))$. From this observation and Lemma 3, we give the next corollary to check the equality between F_{sp} and Feas(Rel(MBP)).

Corollary 1. *Suppose* Feas(Rel(MBP)) *is bounded. Consider* $(P_{\hat{x}})$ *given in* Lemma 3. $F_{sp} = \text{Feas(Rel(MBP))}$ *if and only if* $(P_{\hat{x}})$ *is feasible for all* $\hat{x} \in \mathcal{E}(\text{Feas(Rel(MBP))})$.

Proof. Suppose Feas(Rel(MBP)) is bounded and $F_{sp} = \text{Feas(Rel(MBP))}$. Therefore, assertion follows from Lemma 3. Conversely, suppose $(P_{\hat{x}})$ is feasible for all $\hat{x} \in \mathcal{E}(\text{Feas(Rel(MBP))})$. Then, by Lemma 3, $\hat{x} \in F_{sp}$ for all $\hat{x} \in \mathcal{E}(\text{Feas(Rel(MBP))})$. Since Feas(Rel(MBP)) is bounded, and F_{sp} and Feas(Rel(MBP)) are both convex sets, by Lemma 2,

$$F_{sp} = \text{Feas(Rel(MBP))}.$$

□

Based on Corollary 1, if the feasible region of Rel(MBP) is bounded, one needs to confirm that (P_x) is feasible for all $x \in \mathcal{E}(\text{Feas(Rel(MBP))})$ for reaching the conclusion $F_{sp} = \text{Feas(Rel(MBP))}$. Since Feas(Rel(MBP)) is a polyhedron, it will have finite number of extreme points. However, it still potentially has too many extreme points and therefore this creates a difficulty. In the next sections, depending on the type of the considered outer approximation, we try to overcome this difficulty by giving sufficient (or necessary) conditions for $F_{sp} = \text{Feas(Rel(MBP))}$ or $F_{sp} \subset \text{Feas(Rel(MBP))}$. We close this section with the following two examples illustrating that the inclusion between F_{sp} and Feas(Rel(KP)) can either hold strictly or as equality.

Example 1. *Let*

$$\text{Feas(Rel(MBP))} := \{x \in \mathbb{R}^2 : 2x_1 + x_2 = 3, \quad x_1 + 2x_2 = 3, \quad x \geq 0\}.$$

and $B = \{1, 2\}$. *Observe that* $\text{Feas(Rel(MBP))} = \text{Feas(MBP)} = \{(1,1)\}$. *If write*

$(P_{\hat{x}})$ for $\hat{x} = (1,1)$ and $\mathcal{K} = \mathcal{N}$

$$
\begin{aligned}
(P_{\hat{x}}) \quad \min \quad & 0 \\
\text{s.t.} \quad & 4X_{11} + 4X_{12} + X_{22} = 9, \\
& X_{11} + 4X_{12} + 4X_{22} = 9, \\
& X_{11} = 1, \\
& X_{22} = 1, \\
& \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} \in \mathcal{N},
\end{aligned}
$$

observe that $E \in \mathcal{S}^3$ is a feasible solution for $(P_{\hat{x}})$, where E is the matrix of all ones. This implies $\hat{x} \in F_{sp}$ by Lemma 3. *Therefore, by* Lemma 2, *we conclude that* $\text{Feas}(\text{Rel}(\text{MBP})) = F_{sp}$.

In the next example, we show that the inclusion in the Lemma 2 can also hold strictly.

Example 2. *Let*

$$\text{Feas}(\text{Rel}(\text{MBP})) := \{x \in \mathbb{R}^2 : 2x_1 + x_2 = 1, \quad x_1 + 2x_2 = 1, \quad x \geq 0\}.$$

and $B = \{1,2\}$. Observe that $\text{Feas}(\text{Rel}(\text{MBP})) = \{(1/3, 1/3)\}$ *and* $\text{Feas}(\text{MBP}) = \emptyset$. *If write $(P_{\hat{x}})$ for $\hat{x} = (1/3, 1/3)$ and $\mathcal{K} = \mathcal{N}$*

$$
\begin{aligned}
(P_{\hat{x}}) \quad \min \quad & 0 \\
\text{s.t.} \quad & 4X_{11} + 4X_{12} + X_{22} = 1, \\
& X_{11} + 4X_{12} + 4X_{22} = 1, \\
& X_{11} = 1/3, \\
& X_{22} = 1/3, \\
& \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} \in \mathcal{N},
\end{aligned}
$$

observe that $(P_{\hat{x}})$ *is infeasible since* X_{12} *cannot take a negative value. Therefore, by* Lemma 3, $\hat{x} \notin F_{sp}$. *This implies* $F_{sp} = \emptyset$ *and thus* $F_{sp} \subset \text{Feas}(\text{Rel(MBP)})$ *by* Lemma 2.

3.3 Outer Polyhedral Approximations

In this section, we will establish our results based on the hierarchy of outer polyhedral approximations proposed by de Klerk and Pasechnik [22], which are already described in Chapter 2. More specifically, we will evaluate the relaxations of Burer's reformulation [18] arising from these outer approximations of $\mathcal{CP}$, and compare their feasible regions and optimal values to those of Rel(MBP).

Recall that de Klerk and Pasechnik [22] established

$$\mathcal{CP} \subseteq \ldots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0 = \mathcal{N}, \quad \text{and} \quad \mathcal{CP} = \bigcap_{r \in \mathbb{N}} \mathcal{O}_r \tag{3.9}$$

Let us define the following problems:

$$\begin{aligned} (\text{Out})_r \quad \ell_r := \quad \min \quad & c^T x \\ \text{s.t.} \quad & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\ & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\ & x_j = X_{jj}, \quad j \in B, \\ & \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{O}_r, \end{aligned} \tag{3.10}$$

where $r \in \mathbb{N}$. Observe that $(\text{Out})_r$ is also a *sign preserving outer approximation* since, by (3.9), nonnegativity restriction on $x \in \mathbb{R}^n$ is already implied for all $r \in \mathbb{N}$. Therefore, all results established in Section 3.2 apply to this section as well. Clearly, for a given instance of (MBP), (3.9) implies that

$$\ell_0 \leq \ell_1 \leq \ldots \leq \nu.$$

Furthermore, by Proposition 2, if the dual of (MBP-CP) has a strictly feasible solution and an attainable optimal solution, then

$$\lim_{r\to\infty} \ell_r = \nu. \tag{3.11}$$

3.3.1 Relation Between the Feasible Regions

We define the following set:

$$F_r := \{x \in \mathbb{R}^n : (x, X) \in \text{Feas}(\text{Out})_r\}, \quad r \in \mathbb{N}. \tag{3.12}$$

By Lemma 2, we already know that $F_r \subseteq \text{Feas}(\text{Rel}(\text{MBP}))$ for all $r \in \mathbb{N}$. In the following lemma, we will establish the relations between F_r, Feas(Rel(MBP)) and Conv(Feas(MBP)).

Lemma 4. Feas(Rel(MBP)) $\supseteq F_0 \supseteq F_1 \supseteq \ldots \supseteq$ Conv(Feas(MBP)). *Furthermore, if the dual problem of* (MBP-CP) *has a strictly feasible solution and an attainable optimal solution, then*

$$\bigcap_{r\in N} F_r = \text{Conv}(\text{Feas}(\text{MBP})). \tag{3.13}$$

Proof. Feas(Rel(MBP)) $\supseteq F_0$ is implied by Lemma 2. Also, $F_0 \supseteq F_1 \supseteq \ldots \supseteq$ Conv(Feas(MBP)) follows from (3.9) and Burer's result [18, Corollary 2.4].

We now show that (3.13) is also true under the given assumptions. For a contradiction, suppose (3.13) is not true, which implies that $\bigcap_{r\in N} F_r \supset$ Conv(Feas(MBP)). Then there exists $x \in \bigcap_{r\in N} F_r$ such that $x \notin$ Conv(Feas(MBP)). It is easy to verify that Conv(Feas(MBP)) is a closed set. Therefore, by strict separation (see, e.g., [16]), there also exists a hyperplane that strictly separates x and Conv(Feas(MBP)). Then, by choosing an objective function such that its improving direction is perpendicular to that hyperplane, it can be guaranteed that

$$\ell_r \leq c^T x < \nu,$$

for all $r \in \mathbb{N}$. However, due to Proposition 2, this contradicts with the fact that $\lim_{r\to\infty} \ell_r = \nu$. Therefore, we conclude that (3.13) is true under the given assumption.

□

3.3.2 A Sufficient Condition for the Equality at Level 0

In this section, we will analyze the relation between F_0 and Feas(Rel(MBP)) in more detail, and we will establish a sufficient condition for the equality between these sets.

Note that by (3.9), $\mathcal{O}_0 = \mathcal{N}$. Therefore, as Example 1 and Example 2 illustrate, the inclusion between F_0 and Feas(Rel(MBP)) might hold strictly, i.e., $F_0 \subset$ Feas(Rel(MBP)) or equally, i.e., $F_0 =$ Feas(Rel(MBP)). If one needs to decide whether $F_0 =$ Feas(Rel(MBP)) or not, then due to Lemma 3, feasibility of the following LP problem should be confirmed for all $\hat{x} \in$ Feas(Rel(MBP)):

$$\begin{aligned} \min \quad & 0 \\ \text{s.t.} \quad & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\ & X_{jj} = \hat{x}_j, \quad j \in B, \\ & \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} \in \mathcal{N}, \end{aligned}$$

which can be simplified to

$$\begin{aligned} \min \quad & 0 \\ \text{s.t.} \quad & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\ & X_{jj} = \hat{x}_j, \quad j \in B, \\ & X \in \mathcal{N}, \end{aligned} \tag{3.14}$$

where $X \in \mathcal{S}^n$ is the decision variable. However, this cannot be confirmed by solving for all $\hat{x} \in$ Feas(Rel(MBP)) since Feas(Rel(MBP)) most likely includes infinitely many points. On the other hand, if Feas(Rel(MBP)) is bounded, then, by Corollary 1, it would be sufficient to solve (3.14) only for extreme points of Feas(Rel(MBP)) to decide if $F_0 = \text{Feas(Rel(MBP))}$. However, this is still hardly practical since there might be too many extreme points of Feas(Rel(MBP)). Therefore, in this section, we will establish a useful sufficient condition to confirm the equality of these two sets, namely F_0 and Feas(Rel(MBP)). Moreover, unlike Corollary 1, this result is valid even though the boundedness assumption on Feas(Rel(MBP)) does not hold.

Before that, we will make a last minor modification on (3.14) for the simplicity. Without loss of generality, assume $B = \{1, \ldots, k\}$, where $k \leq n$. Then, (3.14) can be rewritten as

$$\begin{aligned} \min \quad & 0 \\ \text{s.t.} \quad & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\ & X_{jj} = \hat{x}_j, \quad j = 1, \ldots, k, \\ & X \in \mathcal{N}. \end{aligned} \tag{3.15}$$

By Lemma 3, $F_0 = \text{Feas(Rel(MBP))}$ if and only if (3.15) is feasible for all $\hat{x} \in \text{Feas(Rel(MBP))}$. Therefore, we want to find a condition so that (3.15) will be feasible for all $\hat{x} \in \text{Feas(Rel(MBP))}$. To do that, we will utilize the dual problem of (3.15). Now, given an arbitrary $\hat{x} \in \mathbb{R}^n$, the dual problem of (3.15) can be written as

$$\max \quad \theta(w, y) \tag{3.16}$$

where $w \in \mathbb{R}^k$, $y \in \mathbb{R}^m$ and

$$\begin{aligned} \theta(w, y) &= \min_{X \in \mathcal{N}} \left\{ \sum_{i=1}^m y_i \left(b_i^2 - \langle X, a_i {a_i}^T \rangle \right) + \sum_{j=1}^k w_j (\hat{x}_j - X_{jj}) \right\}, \\ &= \sum_{i=1}^m y_i b_i^2 + \sum_{j=1}^k w_j \hat{x}_j + \min_{X \in \mathcal{N}} \left\{ \left\langle X, -\sum_{i=1}^m y_i a_i {a_i}^T \right\rangle - \sum_{j=1}^k w_j X_{jj} \right\}. \end{aligned}$$

Define

$$W := \text{Diag}([w_1 \ldots w_k \; 0 \ldots 0]).$$

Then, $\theta(w, y)$ can be written as follows:

$$\theta(w, y) = \sum_{i=1}^m y_i b_i^2 + \sum_{j=1}^k w_j \hat{x}_j + \min_{X \in \mathcal{N}} \left\{ \left\langle X, -\sum_{i=1}^m y_i a_i {a_i}^T - W \right\rangle \right\}, \tag{3.17}$$

Note that both (3.15) and (3.16) are LP problems. Therefore, if (3.15) is feasible, then, by strong duality, 0 will be the optimal value for both of them. Clearly, from (3.17)

$$\theta(w,y) = \begin{cases} \sum_{i=1}^{m} y_i b_i^2 + \sum_{j=1}^{k} w_j \hat{x}_j, & \text{if } \sum_{i=1}^{m} y_i a_i {a_i}^T + W \leq 0 \\ -\infty, & \text{otherwise} \end{cases}$$

Hence, (3.16) can be rewritten as

$$\begin{aligned} \max \quad & f(w,y) := \sum_{i=1}^{m} y_i b_i^2 + \sum_{j=1}^{k} w_j \hat{x}_j \\ \text{s.t.} \quad & \sum_{i=1}^{m} y_i a_i {a_i}^T + W \leq 0, \end{aligned} \tag{3.18}$$

where $w \in \mathbb{R}^k$ and $y \in \mathbb{R}^m$ are decision variables. Since (3.18) is the dual problem of (3.15) and $(w,y) = (0,0)$ is always a feasible solution for it, one can easily see that (3.18) will either be unbounded or bounded with the optimal value 0. Therefore, (3.15) is feasible if and only if (3.18) is bounded. If we write the constraints of (3.18) that include $w_1, \ldots, w_k$, they are

$$\sum_{i=1}^{m} y_i {(a_i)_j}^2 + w_j \leq 0, \quad j = 1, \ldots, k.$$

Since $\hat{x} \in \text{Feas(Rel(MBP))}$ (and thus $\hat{x} \in \mathbb{R}^n_+$), multiplying them with $\hat{x}_j$ would give us

$$\sum_{i=1}^{m} y_i {(a_i)_j}^2 \hat{x}_j + w_j \hat{x}_j \leq 0, \quad j = 1, \ldots, k.$$

If we sum them up, we get the inequality,

$$\sum_{i=1}^{m} y_i \sum_{j=1}^{k} {(a_i)_j}^2 \hat{x}_j + \sum_{j=1}^{k} w_j \hat{x}_j \leq 0. \tag{3.19}$$

We will try to specify a condition that ensures the implication

$$\sum_{i=1}^{m} y_i \sum_{j=1}^{k} {(a_i)_j}^2 \hat{x}_j + \sum_{j=1}^{k} w_j \hat{x}_j \leq 0 \implies f(w,y) \leq 0.$$

Now, let

$$A := \begin{bmatrix} a_1^T \\ \vdots \\ a_m^T \end{bmatrix} \in \mathbb{R}^{m\times n}. \tag{3.20}$$

Let A_j be the j^{th} column vector of A, $j = 1, \dots, n$. By taking the Hadamard product of each pair of column vector $A_j \circ A_l$ such that $1 \le j < l \le n$ we obtain a matrix $T \in \mathbb{R}^{m\times \binom{n}{2}}$, which is given as follows:

$$T := \begin{bmatrix} A_1 \circ A_2 & \dots & A_1 \circ A_n & A_2 \circ A_3 & \dots & A_{n-1} \circ A_n \end{bmatrix} \tag{3.21}$$

Let, also

$$I^+ := \{i \in \{1, \dots, m\} : a_i \in \mathbb{R}^n_+\} \text{ and } I^- := \{1, \dots, m\} \setminus I^+. \tag{3.22}$$

We will use (3.19), and definitions (3.21) and (3.22) in the proof of following theorem. Next theorem establishes a sufficient condition for the equality of F_0 and Feas(Rel(MBP)).

Theorem 3. *Let T, I^+ and I^- be defined as in (3.21) and (3.22). By changing the order of the rows and columns in T, suppose it can be put into the form*

$$\begin{array}{c} I^+ \\ \hline I^- \end{array} \left[\begin{array}{c|c|c} D_1 & \begin{array}{c} 0 \\ \hline D_2 \end{array} & G \end{array} \right], \tag{3.23}$$

where $D_1 \in \mathbb{R}^{m\times m}$ is a diagonal matrix with strictly positive diagonals, $D_2 \in \mathbb{R}^{|I^-|\times|I^-|}$ is a diagonal matrix with strictly negative diagonals and $G \in \mathbb{R}^{m\times\left(\binom{n}{2} - m - |I^-|\right)}$ is any matrix with no restriction. Then, $F_0 = \text{Feas(Rel(MBP))}$. As a result, $\ell_0 = \ell_{LP}$.

Proof. Suppose T can be put into the form (3.23). Observe that due to the special form of T, we have the following constraints on (3.18):

$$y_i \leq 0, \ \forall i \in I^+ \text{ and } y_i = 0, \ \forall i \in I^-.$$

Recall that (3.19) is also implied by the constraints of (3.18). Observe that (3.19) can be rewritten as

$$\sum_{i \in I^+}^{m} \underbrace{y_i}_{\leq 0} \underbrace{\sum_{j=1}^{k} {(a_i)_j}^2 \hat{x}_j}_{\leq {b_i}^2} + \underbrace{\sum_{i \in I^-}^{m} \underbrace{y_i}_{=0} \sum_{j=1}^{k} {(a_i)_j}^2 \hat{x}_j}_{=0} + \sum_{j=1}^{k} w_j \hat{x}_j \leq 0,$$

which implies that

$$f(w,y) = \sum_{i=1}^{m} y_i b_i^2 + \sum_{j=1}^{k} w_j \hat{x}_j \leq 0,$$

for all $\hat{x} \in \mathbb{R}^n_+$. Since $(w,y) = (0,0)$ is always a feasible solution for (3.18), this implies that the optimal value of (3.18) is 0 for all $\hat{x} \in \mathbb{R}^n_+$. This also implies (3.15) is feasible for all $\hat{x} \in \mathbb{R}^n_+$. Therefore, by Lemma 3, we conclude that $F_0 = \text{Feas(Rel(MBP))}$. □

Remark 1. *Observe that T can be put into the form* (3.23) *if and only if both of the following conditions hold:*

(i) For each $i \in \{1, \ldots, m\}$, there exists (j,l), $j \neq l$, such that ${(a_i)}_j . {(a_i)}_l > 0$ and ${a^p}_j . {a^p}_l = 0$, for all $p = 1, \ldots, m$, $p \neq i$.

(ii) For each $i \in I^-$, there exists (j,l), $j \neq l$, such that ${(a_i)}_j . {(a_i)}_l < 0$ and ${a^p}_j . {a^p}_l = 0$, for all $p = 1, \ldots, m$, $p \neq i$.

We next give an example, in which T defined in (3.21) can be put into the form (3.23).

Example 3. *Consider an instance of* (MBP)*. Let*

$$\begin{aligned} {a_1}^T &= \begin{bmatrix} 0 & 2 & 0 & 4 & 0 \end{bmatrix}, \\ {a_2}^T &= \begin{bmatrix} 1 & 3 & 0 & 0 & 0 \end{bmatrix}, \\ {a_3}^T &= \begin{bmatrix} 4 & 0 & 0 & -1 & 2 \end{bmatrix}, \\ {a_4}^T &= \begin{bmatrix} 0 & 5 & -2 & 0 & 1 \end{bmatrix}. \end{aligned} \tag{3.24}$$

For brevity, we will not write the other problem parameters, since (3.23) *in* Theorem 3 *depends only on* a_i*,* $i = 1, \ldots, m$*. Now,* A *defined in* (3.20) *is*

$$A = \begin{bmatrix} 0 & 2 & 0 & 4 & 0 \\ 1 & 3 & 0 & 0 & 0 \\ 4 & 0 & 0 & -1 & 2 \\ 0 & 5 & -2 & 0 & 1 \end{bmatrix}.$$

Accordingly, T *defined in* (3.21) *is*

$$T = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 8 & 0 & 0 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & -10 & 0 & 5 & 0 & -2 & 0 \end{bmatrix}.$$

By changing the order of the columns of T*, observe that it can be put into the form* (3.23) *as follows:*

$$\begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & -4 & 0 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 5 & 0 & -2 & 0 & 0 & -10 & 0 \end{bmatrix},$$

where

$$D_1 = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 5 \end{bmatrix}, D_2 = \begin{bmatrix} -4 & 0 \\ 0 & -2, \end{bmatrix} \text{ and } G = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & -10 & 0. \end{bmatrix}$$

Hence, if an (MBP) *instance consists of the vectors* a_i*,* $i = 1, \ldots, 4$*, given in* (3.24)*, then, by* Theorem 3*,* $F_0 = \text{Feas}(\text{Rel}(\text{MBP}))$ *holds regardless of the other problem parameters and therefore* $\ell_0 = \ell_{LP}$*.*

We close this section with the following example showing that the sufficient condition given in Theorem 3 cannot be relaxed, in general.

Example 4. *Consider the following instance of* (MBP)*:*

$$
\begin{gathered}
c^T = \begin{bmatrix} 4 & -6 & -2 & 0 & 0 \end{bmatrix}, \\
{a_1}^T = \begin{bmatrix} 9 & 1 & 1 & 0 & 0 \end{bmatrix} \\
{a_2}^T = \begin{bmatrix} 10 & -1 & -1 & 0 & 0 \end{bmatrix} \\
{a_3}^T = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \end{bmatrix} \\
{a_4}^T = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \end{bmatrix} \\
b^T = \begin{bmatrix} 9.1 & 9.9 & 1 & 1 \end{bmatrix} \\
x_1, x_2 \in \{0, 1\}, \\
x_3, x_4, x_5 \geq 0.
\end{gathered}
$$

Observe that (i) in Remark 1 *is violated and thus* T *cannot be put into the form* (3.23)*. Optimal values and optimal solutions of* (MBP)*,* Rel(MBP) *and* $(\text{Out})_0$ *respectively, are as follows:*

$$
\begin{gathered}
\nu = 3.8, \quad x^{*T} = \begin{bmatrix} 1 & 0 & 0.1 & 0 & 1 \end{bmatrix} \\
\ell_{LP} = 3.4, \quad {x_{bin}^*}^T = \begin{bmatrix} 1 & 0.1 & 0 & 0 & 0.9 \end{bmatrix} \\
\ell_0 = 3.76, \quad x_0^{*T} = \begin{bmatrix} 1 & 0.01 & 0.09 & 0 & 0.99 \end{bmatrix}, \quad X_0^* = \begin{bmatrix} 1 & 0 & 0.1 & 0 & 0 \\ 0 & 0.01 & 0 & 0 & 0 \\ 0.1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.99 \end{bmatrix}
\end{gathered}
$$

Hence $\ell_0 > \ell_{LP}$*, which implies that* $F_0 \subset \text{Feas}(\text{Rel}(\text{MBP}))$*.*

3.3.3 Higher Levels

Note that throughout this section we assume that dual problem of (MBP-CP) has a strictly feasible solution and an attainable optimal solution. Therefore, (3.13) holds. Given $\hat{x} \in \text{Feas}(\text{Rel}(\text{MBP}))$, there are two possible cases: either $\hat{x} \in \text{Conv}(\text{Feas}(\text{MBP}))$ or otherwise. In the first case, by Lemma 4, $\hat{x} \in F_r$ for all $r \in \mathbb{N}$. Otherwise, if the dual problem of (MBP-CP) has an attainable optimal solution and a strictly feasible solution, then due to Lemma 4, it is certain that there exists $r_0 \in \mathbb{N}$ such that $x \in F_r$ for all $r < r_0$ and $x \notin F_r$ for all $r \geq r_0$. Let us define

$$F^-_{Rel} := \text{Feas}(\text{Rel}(\text{MBP})) \setminus \text{Conv}(\text{Feas}(\text{MBP})). \tag{3.25}$$

Given $\hat{x} \in F^-_{Rel}$, one can always solve $(P_{\hat{x}})$ in Lemma 3 to check if $\hat{x} \in F_r$ or not at any level $r \in \mathbb{N}$. Moreover, $(P_{\hat{x}})$ gives an LP problem when $\mathcal{K} = \mathcal{O}_r$. However, observe that its size grows exponentially with respect to r. In this section, we will investigate until at least what level $r \in \mathbb{N}$, $\hat{x} \in F_r$ holds, and after at most what level $r \in \mathbb{N}$, $\hat{x} \notin F_r$ holds.

First, we will give a sufficient condition, under which $\hat{x} \in F_r$ holds until at least a certain level of r. Next, at any level $r \in \mathbb{N}$, we will give a necessary condition for $\hat{x} \in F_r$. What makes our conditions useful is that computational effort required to check them does not change depending on the level $r \in \mathbb{N}$ at all.

A Sufficient condition

We first present our sufficient condition. Suppose $\hat{x} \in F^-_{Rel}$ consists of only rational elements, i.e., $\hat{x} \in \mathbb{Q}^n$. Then, there obviously exists $k \in \mathbb{N}$ such that $k\hat{x} \in \mathbb{N}^n$. Let $u^T := \begin{bmatrix} k+1 & k\hat{x}^T \end{bmatrix} \in \mathbb{N}^{n+1}$. Let

$$M := \frac{1}{k(k+1)}(uu^T - \text{Diag}(u)) = \begin{bmatrix} 1 & \hat{x} \\ \hat{x}^T & \frac{1}{k+1}(k\hat{x}\hat{x}^T - \text{Diag}(\hat{x})) \end{bmatrix}$$

Observe that $M \in \mathcal{O}_r$ until at least $r = (k-1) + ke^T\hat{x}$. Let us define another matrix

$$\bar{M} := M + \mathrm{Diag}(y), \tag{3.26}$$

where $y \in \mathbb{R}^{n+1}$ is such that $y_1 = 0$, $y_{j+1} = \left(\frac{k+2}{k+1}\right)\hat{x}_j - \left(\frac{k}{k+1}\right)\hat{x}_j^2$ for $j \in B$ and $y_{j+1} = 0$ for $j \in \{1,\dots,n\} \setminus B$. Observe that $\bar{M} \in \mathcal{O}_r$ until at least $r = (k-1)+ke^T\hat{x}$ as well. Also, the diagonal entries of $\bar{M}$ satisfy $\bar{M}_{j+1,j+1} = \hat{x}_j$ for all $j \in B$.

Let $\mathcal{H} := \{2,\dots,n+1\}$. Consider an instance of (MBP). Then,

$$\begin{aligned}
{a_i}^T\bar{M}[\mathcal{H}]a_i &= {a_i}^T M[\mathcal{H}]a_i + {a_i}^T(\mathrm{Diag}(y)[\mathcal{H}])a_i \\
&= \left\langle a_i a_i^T, \frac{1}{k+1}\left(k\hat{x}\hat{x}^T - \mathrm{Diag}(\hat{x})\right)\right\rangle + \sum_{j\in B}{(a_i)_j}^2\left(\frac{k+2}{k+1}\hat{x}_j - \frac{k}{k+1}\hat{x}_j^2\right) \\
&= \frac{k}{k+1}b_i^2 - \sum_{j=1}^{n}\frac{1}{k+1}{(a_i)_j}^2\hat{x}_j + \sum_{j\in B}{(a_i)_j}^2\left(\frac{k+2}{k+1}\hat{x}_j - \frac{k}{k+1}\hat{x}_j^2\right) \\
&= \frac{k}{k+1}b_i^2 + \sum_{j\in B}{(a_i)_j}^2\hat{x}_j - \sum_{j\in\{1,\dots,n\}\setminus B}\frac{1}{k+1}{(a_i)_j}^2\hat{x}_j - \sum_{j\in B}\frac{k}{k+1}{(a_i)_j}^2\hat{x}_j^2
\end{aligned}$$

for $i = 1,\dots,m$. Therefore,

$$b_i^2 - {a_i}^T\bar{M}[\mathcal{H}]a_i = \frac{1}{k+1}\left(b_i^2 + \sum_{j\in\{1,\dots,n\}\setminus B}{(a_i)_j}^2\hat{x}_j\right) - \sum_{j\in B}{(a_i)_j}^2\left(\hat{x}_j - \frac{k}{k+1}\hat{x}_j^2\right),$$

$i = 1,\dots,m$. If we define the following,

$$\zeta_i := b_i^2 + \sum_{j\in\{1,\dots,n\}\setminus B}{(a_i)_j}^2\hat{x}_j, \quad i = 1,\dots,m, \tag{3.27}$$

$$\mu_i := \sum_{j\in B}{(a_i)_j}^2\left(\hat{x}_j - \frac{k}{k+1}\hat{x}_j^2\right), \quad i = 1,\dots,m, \tag{3.28}$$

Observe that

$$b_i^2 - {a_i}^T\bar{M}[\mathcal{H}]a_i = \frac{\zeta_i}{k+1} - \mu_i. \tag{3.29}$$

In the following theorem, we construct a matrix $\tilde{M}$ that fills the gap (3.29) and whose x-component is equal to $\hat{x}$. It also satisfies $\tilde{M} \in \mathrm{Feas(Out)}_r$ until at least $r = (k-1) + ke^T\hat{x}$. The construction of such a matrix becomes possible by an LP problem with m constraints and only $n - |B|$ variables given in (3.30).

Theorem 4. *Let $\hat{x} \in F^-_{Rel}$. Suppose $\hat{x} \in \mathbb{Q}^n$ and let $k \in \mathbb{N}$ such that $k\hat{x} \in \mathbb{N}^n$. Let ζ_i and μ_i be defined as in* (3.27) *and* (3.28)*. Suppose there exists a feasible solution to the following LP problem*

$$\begin{aligned} \min \quad & 0 \\ \text{s.t.} \quad & \sum_{j \in \{1,\ldots,n\} \setminus B} {(a_i)_j}^2 w_j = \frac{\zeta_i}{k+1} - \mu_i, \quad i = 1, \ldots, m, \\ & w_j \geq 0, \quad j \in \{1, \ldots, n\} \setminus B, \end{aligned} \tag{3.30}$$

where w_j, $j \in \{1, \ldots, n\} \setminus B$ are decision variables. Then $\hat{x} \in F_r$, until at least $r = (k-1) + ke^T\hat{x}$.

Proof. Suppose $\hat{w}_j$, $j \in \{1, \ldots, n\} \setminus B$, is a feasible solution to problem (3.30). Let $\bar{M}$ be defined as in (3.26). Define $z \in \mathbb{R}^{n+1}$ such that $z_1 = 0$, $z_{j+1} = \hat{w}_j$ for $j \in \{1, \ldots, n\} \setminus B$ and $z_{j+1} = 0$ for $j \in B$. Let us define $\tilde{M} := \bar{M} + \text{Diag}(z)$. Observe that $\tilde{M} \in \mathcal{O}_r$, until at least $r = (k-1) + ke^T\hat{x}$. If we write $\tilde{M}$ in more explicit form

$$\tilde{M} = \begin{bmatrix} 1 & \hat{x} \\ \hat{x}^T & \frac{1}{k+1}(k\hat{x}\hat{x}^T - \text{Diag}(\hat{x})) \end{bmatrix} + \text{Diag}(y) + \text{Diag}(z).$$

Since x-component of $\tilde{M}$ is $\hat{x}$, $\tilde{M}$ satisfies first set of m constraints in $(\text{Out})_r$. Recall that $\mathcal{H} := \{2, \ldots, n+1\}$. Now, observe that

$$\begin{aligned} a_i^T \tilde{M}[\mathcal{H}] a_i &= a_i^T \bar{M}[\mathcal{H}] a_i + a_i^T \text{Diag}(z) a_i \\ &= a_i^T \bar{M}[\mathcal{H}] a_i + \sum_{j \in \{1,\ldots,n\} \setminus B} {(a_i)_j}^2 \hat{w}_j \\ &= a_i^T \bar{M}[\mathcal{H}] a_i + \frac{\zeta_i}{k+1} - \mu_i \end{aligned}$$

for $i = 1, \ldots, m$. Therefore, by (3.29), $a_i^T \tilde{M}[\mathcal{H}] a_i = b_i^2$, which implies that $\tilde{M}$ satisfies second set of m constraints in $(\text{Out})_r$. Also, observe that the diagonal entries $\tilde{M}_{j+1,j+1} = \hat{x}_j$, for all $j \in B$. Therefore $\tilde{M} \in \text{Feas}(\text{Out})_r$, which implies that $\hat{x} \in F_r$, until at least $r = (k-1) + ke^T\hat{x}$. This completes the proof. □

Remark 2. *Observe that problem* (3.30) *can possibly be infeasible due to following two reasons: Firstly, it has a linear system of equations (l.s.e) with m equations and $n - |B|$ variables. It is likely that the l.s.e is overdetermined if $m > n - |B|$. Secondly, its variables have nonnegativity restriction and it is not guaranteed that $\frac{\zeta_i}{k+1} - \mu_i \geq 0$, $i = 1, \dots, m$. Since each w_j, $j = \{1, \dots, n\} \setminus B$ is multiplied by ${(a_i)_j}^2$, if there exists $i \in \{1, \dots, m\}$ such that $\frac{\zeta_i}{k+1} - \mu_i < 0$, then* (3.30) *again becomes infeasible. Therefore, in all these cases* Theorem 4 *remains inconclusive. However, an advantage of* Theorem 4 *is that* (3.30) *is an LP problem and its size* (3.30) *is not dependent on the level $r \in \mathbb{N}$.*

Following example includes an (MBP) instance, for which we can reach to a conclusion by using Theorem 4.

Example 5. *Consider the following* (MBP) *instance.*

$$\begin{gathered} c^T = \begin{bmatrix} -1 & 0 & 1 & 0 \end{bmatrix} \\ {a_1}^T = \begin{bmatrix} 1 & 1 & 1 & 4 \end{bmatrix}, \\ {a_2}^T = \begin{bmatrix} 1 & 3 & 4 & 5 \end{bmatrix}, \\ b^T = \begin{bmatrix} 1 & 2 \end{bmatrix}, \\ x \geq 0, \\ x_1 \in \{0, 1\}. \end{gathered}$$

Optimal values and optimal solutions of (MBP) *and* Rel(MBP) *are respectively as follows:*

$$\begin{gathered} \nu = 0, \quad x^{*T} \approx \begin{bmatrix} 0 & 0.4286 & 0 & 0.1429 \end{bmatrix}, \\ \ell_{LP} = -0.5, \quad {x^*_{bin}}^T = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 \end{bmatrix} \in F^-_{Rel}. \end{gathered}$$

Note that Rel(MBP) *has a unique optimal solution. Let $\hat{x} = x^*_{bin}$. Observe that $k\hat{x} \in \mathbb{N}$ for $k = 2, 4, 6, \dots$. If we solve* (3.30) *for this instance, it continues to be* *feasible until $k = 8$, which implies that $\hat{x} \in F_r$, until at least $r = (k-1) + ke^T\hat{x} = 15$. Therefore, we conclude that $\ell_r = \ell_{LP} = -0.5$ for all $r = 0, 1, \ldots, 15$. However, if we solve $(\text{Out})_r$ for this problem, it turns out that $\ell_r = \ell_{LP} = -0.5$ until $r = 112$, and $\ell_{113} = -0.4674$.*

This example is important since it shows that for the considered instance, the lower bound given by $(\text{Out})_r$ does not improve until $r = 112$. However, at $r = 112$, the resulting LP problem has $7,673,835$ variables! Although the number of variables increased dramatically and more than 7 million variables are added to $(\text{Out})_r$ starting from $r = 0$ to $r = 112$, the resulting lower bound does not improve. This is obviously not a desired result for outer approximations. Moreover, our computational efforts indicate that this is not uncommon among (MBP) instances.

In Chapter 4, we will also establish important theoretical results for the 0-1 knapsack problem which is a special case of (MBP). Those results will also show that lower bounds resulting from $(\text{Out})_r$ do not improve until at least a certain level of $r \in \mathbb{N}$ for the 0-1 knapsack problem.

Given $\hat{x} \in F_{Rel}^{-}$, in Theorem 4, we established a sufficient condition that ensures $\hat{x} \in F_r$ until at least a certain level $r \in \mathbb{N}$. Now, we will establish a necessary condition that holds true if $\hat{x} \in F_r$.

A Necessary Condition

Given $\hat{x} \in F_{Rel}^{-}$ and level $r \in \mathbb{N}$, suppose $\hat{x} \in F_r$, which implies there exists $M \in \text{Feas}(\text{Out})_r$ such that

$$M = \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} = \sum_{z \in \Theta(n+1,r)} \lambda_z (zz^T - \text{Diag}(z)), \tag{3.31}$$

where $\lambda_z \geq 0$ for all $z \in \Theta(n+1, r)$. We can partition $z \in \Theta(n+1, r)$ so that

$$z^T = \left[\begin{array}{c|c} z_0 & {z_1}^T \end{array}\right] \tag{3.32}$$

where $z_0 \in \mathbb{N}$ and $z_1 \in \mathbb{N}^n$. Now, let us define the following two sets:

$$S_1 := \{z \in \Theta(n+1,r) : z_0 \geq 1\},$$
$$S_2 := \{z \in \Theta(n+1,r) : z_0 = 0\}.$$

Obviously $S_1 \cap S_2 = \emptyset$ and $S_1 \cup S_2 = \Theta(n+1,r)$. Now suppose $|\Theta(n+1,r)| = p$, $|Z_1| = h$ and w.l.o.g. assume first h vectors of $\Theta(n+1,r)$, i.e., z^k, $k = 1,\ldots,h$, are in the set S_1 and the remaining vectors of $\Theta(n+1,r)$, i.e., z^k, $k = h+1,\ldots,p$, are in the set S_2. Since $M \in \text{Feas(Out)}_r$, we can write the following equalities resulting from (3.31):

$$\sum_{k=1}^{h} \lambda_k \left((z_0^k)^2 - {z_0}^k \right) = 1 \tag{3.33}$$

$$\sum_{k=1}^{h} \lambda_k \left(z_0^k (z_1^k)_j \right) = \hat{x}_j, \quad j = 1,\ldots,n, \tag{3.34}$$

$$\underbrace{\sum_{k=1}^{h} \lambda_k \left({(z_1^k)_j}^2 - (z_1^k)_j \right)}_{=Y_{jj}} + \underbrace{\sum_{k=h+1}^{p} \lambda_k \left({(z_1^k)_j}^2 - (z_1^k)_j \right)}_{\geq 0} = X_{jj}, \quad j = 1,\ldots,n. \tag{3.35}$$

$$\underbrace{\sum_{k=1}^{h} \lambda_k \left((z_1^k)_j (z_1^k)_l \right)}_{=Y_{jl}} + \underbrace{\sum_{k=h+1}^{p} \lambda_k \left((z_1^k)_j (z_1^k)_l \right)}_{\geq 0} = X_{jl}, \quad 1 \leq j < l \leq n. \tag{3.36}$$

In the next lemma, we will establish a result that will be useful for the following theorem.

Lemma 5. *For all $z \in \Theta(n+1,r)$, consider* (3.32), (3.33) *and* (3.34).

$$\sum_{k=1}^{h} \lambda_k z_0^k = \frac{e^T \hat{x} + 1}{r+1},$$

where $e \in \mathbb{R}^n$ is the vector of all ones.

Proof. If we sum (3.34) over all $j = 1, \ldots, n$,

$$\begin{aligned} e^T\hat{x} &= \sum_{j=1}^{n}\sum_{k=1}^{h}\lambda_k\left(z_0^k(z_1^k)_j\right), \\ &= \sum_{k=1}^{h}\lambda_k z_0^k \underbrace{\sum_{j=1}^{n}(z_1^k)_j}_{=r+2-{z_0}^k}, \\ &= (r+2)\left(\sum_{k=1}^{h}\lambda_k z_0^k\right) - \sum_{k=1}^{h}\lambda_k(z_0^k)^2, \\ &= (r+1)\left(\sum_{k=1}^{h}\lambda_k z_0^k\right) - 1. \end{aligned}$$

Then, $\sum_{k=1}^{h}\lambda_k z_0^k = \frac{e^T\hat{x}+1}{r+1}$. □

Before giving our next result, we will make two more definitions. Let

$$\alpha_{\hat{x}} := \frac{e^T\hat{x}+1}{r+1}, \tag{3.37}$$

where $e \in \mathbb{R}^n$ is the vector of all ones and

$$\mathcal{Q}^n = \left\{x \in \mathbb{R}^n : 2x_1x_2 \geq x_3^2 + \cdots + x_n^2, \quad x_1, x_2 \geq 0\right\}. \tag{3.38}$$

Note that $\mathcal{Q}^n$ is a second-order cone. Given $\hat{x} \in F_{Rel}^-$, next theorem establishes that if $\hat{x} \in F_r$, then it is possible to define a problem which includes two different types of conic constraints and a nonempty feasible region. Note that the size of this problem also does not change depending on the level $r \in \mathbb{N}$.

Theorem 5. *Suppose I^+ defined in* (3.22) *is nonempty. Let $\hat{x} \in F_{Rel}^-$, where F_{Rel}^- is* *defined as in* (3.25)*. If $\hat{x} \in F_r$, $r \in \mathbb{N}$, then the following problem is feasible:*

$$
\begin{aligned}
(DC) \quad \min \quad & 0 \\
\text{s.t.} \quad & \sum_{j=1}^{n} {(a_i)_j}^2 w_j + \sum_{j=1}^{n-1} \sum_{l=j+1}^{n} 2(a_i)_j (a_i)_l Z_{jl} \le {b_i}^2, \quad i \in I^+, && (3.39) \\
& Z_{jl} = 0, \quad l = 1, \dots, n; \ j : \hat{x}_j = 0, && (3.40) \\
& Z_{jj} \le w_j, \quad j = 1 \dots, n, && (3.41) \\
& w_j = \hat{x}_j, \quad j \in B, && (3.42) \\
& \eta \ge 0, && (3.43) \\
& (1/2\alpha_{\hat{x}}, (Z_{jj} + \eta_j), \eta_j) \in \mathcal{Q}^3, \quad j = 1, \dots, n, && (3.44) \\
& \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & Z \end{bmatrix} + \text{Diag}\left(\begin{bmatrix} \alpha_{\hat{x}} \\ \eta_1 \\ \vdots \\ \eta_n \end{bmatrix} \right) \in \mathcal{DN}. && (3.45)
\end{aligned}
$$

where $w \in \mathbb{R}^n$, $Z \in \mathbb{R}^{n \times n}$, $\eta \in \mathbb{R}^n$ are decision variables, and $\alpha_{\hat{x}}$ is defined in (3.37)*.*

Proof. Suppose $\hat{x} \in F^-_{Rel}$. If $\hat{x} \in F_r$, then we know that there exists $M \in \text{Feas(Out)}_r$ such that (3.31) holds. Let us define

$$
\begin{aligned}
\bar{z_0^k} &:= \sqrt{\lambda_k} z_0^k, \quad k = 1, \dots, |\Theta(n+1, r)|, \\
(\bar{z_1^k})_j &:= \sqrt{\lambda_k} (z_1^k)_j, \quad k = 1, \dots, |\Theta(n+1, r)|, \ j = 1, \dots, n.
\end{aligned}
$$

Due to (3.33), (3.34), (3.35), (3.36) and Lemma 5,

$$
\begin{aligned}
& \sum_{k=1}^{h} (\bar{z_0^k})^2 = 1 + \alpha_{\hat{x}}, \\
& \sum_{k=1}^{h} \bar{z_0^k} (\bar{z_1^k})_j = \hat{x}_j, \quad j = 1, \dots, n, \\
& \sum_{k=1}^{h} {(\bar{z_1^k})_j}^2 = Y_{jj} + \beta_j, \quad \text{where } \beta_j = \sum_{k=1}^{h} \lambda_k (z_1^k)_j, \quad j = 1, \dots, n, \\
& \sum_{k=1}^{h} (\bar{z_1^k})_j (\bar{z_1^k})_l = Y_{jl} \quad 1 \le j < l \le n.
\end{aligned}
$$

Define the following vectors:

$$u^T := \begin{bmatrix} \bar{z_0^1} & \dots & \bar{z_0^h} \end{bmatrix},$$
$$(v^j)^T := \begin{bmatrix} (\bar{z_1^1})_j & \dots & (\bar{z_1^h})_j \end{bmatrix}, \quad j = 1, \dots, n,$$

Then,

$$\begin{aligned} 1 + \alpha_{\hat{x}} &= u^T u, \\ \hat{x}_j &= u^T v^j, \quad j = 1, \dots, n, \\ Y_{jj} + \beta_j &= (v^j)^T v^j, \quad j = 1, \dots, n, \\ Y_{jl} &= (v^j)^T v^l, \quad 1 \leq j < l \leq n. \end{aligned}$$

Accordingly, if $G := \begin{bmatrix} u & v^1 & \dots & v^n \end{bmatrix} \begin{bmatrix} u & v^1 & \dots & v^n \end{bmatrix}^T$, then

$$G = \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & Y \end{bmatrix} + \mathrm{Diag}\left(\begin{bmatrix} \alpha_{\hat{x}} \\ \beta_1 \\ \vdots \\ \beta_n \end{bmatrix} \right)$$

and it is completely positive by definition. Let $\Lambda := \begin{bmatrix} \sqrt{\lambda_1} & \dots & \sqrt{\lambda_h} \end{bmatrix}$. Recall that $\beta_j = \sum_{k=1}^{h} \lambda_k (z_1^k)_j$. Then,

$$\begin{aligned} \beta_j &= \Lambda^T v^j, \quad j = 1, \dots, n \\ &= \|\Lambda\| \|v^j\| \cos(\mathrm{ang}(v^j, \Lambda)), \quad j = 1, \dots, n \end{aligned}$$

where $\mathrm{ang}(\cdot, \cdot)$ denotes the angle between two given vectors. Observe that

$$\|\Lambda\|^2 = \sum_{k=1}^{h} \lambda^k \leq \sum_{k=1}^{h} \lambda^k \underbrace{{z_0}^k}_{\geq 1} = \alpha_{\hat{x}} \implies \|\Lambda\| \leq \sqrt{\alpha_{\hat{x}}},$$

Therefore,

$$\begin{aligned} \beta_j &= \underbrace{\|\Lambda\|}_{\leq \sqrt{\alpha_{\hat{x}}}} \|v^j\| \underbrace{\cos(\mathrm{ang}(v^j, \Lambda))}_{\leq 1}, \\ &\leq \sqrt{\alpha_{\hat{x}} (Y_{jj} + \beta_j)}, \end{aligned} \tag{3.46}$$

since $\|v^j\|^2 = Y_{jj} + \beta_j$, $j = 1, \ldots, n$. Now, we will show that $(w, Z, \eta) = (\text{diag}(X), Y, \beta)$ is a feasible solution for (DC), where $X = M[\{2, \ldots, n+1\}]$. Since $M \in \text{Feas(Out)}_r$, ${a_i}^T X a_i = b_i^2$, $i = 1, \ldots, m$. Therefore (3.39) holds since $Y \leq X$. If $\hat{x}_j = 0$ for any $j \in \{1, \ldots, n\}$, then, due to (3.34) and (3.36), $Y_{jl} = 0$ since $z_0^k \geq 1$ for all $k = 1, \ldots, h$. Hence, (3.40) is satisfied as well. Due to (3.35), $Y_{jj} \leq X_{jj}$ and thus (3.41) is satisfied. Since $X_{jj} = \hat{x}_j$, (3.42) is satisfied. Since $\beta_j \geq 0$, $j = 1, \ldots, n$, (3.43) is satisfied. Due to (3.46), (3.44) is satisfied. Lastly, since $G \in \mathcal{CP}$ and $\mathcal{CP} \subseteq \mathcal{DN}$, (3.45) is satisfied. Finally, we conclude that $(\text{diag}(X), Y, \beta_j)$ is a feasible solution to (DC). □

Remark 3. *(DC) is a conic optimization problem with two types of conic constraints, $n^2 + n$ variables and less than $|I^+| + (|B| + 2)n + |B|$ constraints. By taking the contraposition of the assertion in* Theorem 5*, if (DC) is infeasible, then it follows that $\hat{x} \notin F_r$.*

Example 6. *Consider the instance of* (MBP) *given in* Example 5*. Starting from $r = 0$, if we solve (DC) for $\hat{x} = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 \end{bmatrix}$ and increase r until it becomes infeasible, observe that it first becomes infeasible at $r = 2151$. This implies $\hat{x} \notin F_{2151}$, although from Example 5 we know that smallest level r such that $\hat{x} \notin F_r$ is equal to 113.*

3.4 Doubly Nonnegative Relaxations

Recall that the *doubly nonnegative cone* is equal to the intersection of the positive semidefinite and nonnegative cones, i.e., $\mathcal{DN} = \mathcal{PSD} \cap \mathcal{N}$. We define the following problem:

$$
\begin{aligned}
\text{(DN)} \quad \ell_{DN} := \quad \min \quad & c^T x \\
\text{s.t.} \quad & {a_i}^T x = b_i, \quad i = 1, \ldots, m, \\
& {a_i}^T X a_i = {b_i}^2, \quad i = 1, \ldots, m, \\
& x_j = X_{jj}, \quad j \in B, \\
& \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{DN}.
\end{aligned} \tag{3.47}
$$

Since $\mathcal{DN} \supseteq \mathcal{CP}$ and the nonnegativity restriction on $x \in \mathbb{R}^n$ is implied by the conic constraint, (DN) is another *sign preserving outer approximation* of (MBP-CP). Hence, all the results established in Section 3.2 will apply to this section as well. Unlike $\mathcal{CP}$, $\mathcal{DN}$ is a tractable cone in the sense that it admits polynomial-time membership oracles. Therefore, (DN) can theoretically be solved in polynomial-time in general. In this section, our aim is to compare the feasible regions and optimal values of the problems (DN) and Rel(MBP). Before beginning our comparison, we shall state the clear relationship between the feasible regions and optimal values of (DN) and $(\text{Out})_0$. Observe that the only difference between these two problems is their conic constraints. (DN) has $\begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{DN}$, whereas $(\text{Out})_0$ has $\begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{N}$. Since $\mathcal{DN} \subseteq \mathcal{N}$, obviously $\text{Feas(DN)} \subseteq \text{Feas}(\text{Out})_0$ and thus $\ell_{DN} \geq \ell_0$.

3.4.1 Comparison of the Feasible Regions

Let us define the following set:

$$
F_{DN} := \{x \in \mathbb{R}^n : (x, X) \in \text{Feas(DN)}\}. \tag{3.48}
$$

By Lemma 2, we already know that $F_{DN} \subseteq \text{Feas(Rel(MBP))}$ and thus $\ell_{DN} \geq \ell_{LP}$. Given $\hat{x} \in \text{Feas(Rel(MBP))}$, to determine whether $\hat{x} \in F_{DN}$ or not, one needs to solve the following by Lemma 3:

$$\begin{aligned} \min \quad & 0 \\ \text{s.t.} \quad & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \dots, m, \\ & X_{jj} = \hat{x}_j, \quad j \in B, \\ & \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & X \end{bmatrix} \in \mathcal{DN}. \end{aligned} \tag{3.49}$$

By Lemma 3, we know that $\hat{x} \in F_{DN}$ if and only if (3.49) is feasible.

We will show that, as long as $\hat{x}[B]$ has 0 or 1 in some of its entries, this problem can be reduced to an equivalent problem of smaller dimension. To make it easier to understand, w.l.o.g. assume that $B = \{1, \dots, k\}$. Also, w.l.o.g. assume $\hat{x}_1 = \ldots = \hat{x}_t = 1$ and $\hat{x}_{t+1} = \ldots = \hat{x}_p = 0$, $p \leq k$. Obviously $0 < x_j < 1$ for $j = p+1, \dots, k$. Let $N := \{1, \dots, n\}$ and $P := \{1, \dots, p\} \subseteq B$.

$$N := \{1, \dots, n\}, \tag{3.50}$$

$$P := \{1, \dots, p\} \subseteq B, , \tag{3.51}$$

$$v_i := a_i[N \setminus P] \in \mathbb{R}^{(n-p)}, \quad i = 1, \dots, m, \tag{3.52}$$

$$w := \hat{x}[N \setminus P] \in \mathbb{R}^{(n-p)}. \tag{3.53}$$

Note that throughout Section 3.4.1, these assumptions will be made. Under these assumptions, we give the following lemma.

Lemma 6. *Given $\hat{x} \in \text{Feas(Rel(MBP))}$, let v_i, $i = 1, \dots, m$ and w be defined as in* (3.52) *and* (3.53)*. $\hat{x} \in F_{DN}$ if and only if the following problem is feasible:*

$$\begin{aligned} (P_{\hat{x}}^{DN}) \quad \min \quad & 0 \\ \text{s.t.} \quad & {v_i}^T X v_i = 0, \quad i = 1, \dots, m, \\ & X_{jj} = w_j(1 - w_j), \quad j = 1, \dots, k-p, \\ & ww^T + X \in \mathcal{N}, \\ & X \in \mathcal{PSD}, \end{aligned}$$

where $X \in \mathcal{S}^{(n-p)}$ is the decision variable.

Proof. We will show that for every feasible solution to (3.49), there exists a feasible solution to $(P_{\hat{x}}^{DN})$ and vice versa. Suppose $M := \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & \hat{X} \end{bmatrix}$ is a feasible solution to (3.49) . We can always write M as

$$M = \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & \hat{X} \end{bmatrix} = \begin{bmatrix} 1 & \hat{x}^T \\ \hat{x} & \hat{x}\hat{x}^T \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & U \end{bmatrix}.$$

Since $M \in \mathcal{DN}$, $U = \left(\hat{X} - \hat{x}\hat{x}^T\right) \in \mathcal{PSD}$. Now, will show that $U[N \setminus P] \in \text{Feas}(P_{\hat{x}}^{DN})$. From the second constraint of (3.49), we know that $\hat{X}_{jj} = \hat{x}_j$, $j \in B$. Since $\hat{x}_j$ is either 0 or 1 for $j \in P$, observe that $\hat{X}_{jj} = \hat{x}_j = \hat{x}_j^2$, $j \in P$. Since $U_{jj} = \hat{X}_{jj} - \hat{x}_j^2$, $j \in N$, this implies $U_{jj} = 0$, for $j \in P$. Since $U \in \mathcal{PSD}$, this implies that first p columns and rows of U are equal to all 0. Therefore,

$$\begin{aligned} {v_i}^T U[N \setminus P] v_i &= {a_i}^T U a_i, \\ &= {a_i}^T \left(\hat{X} - \hat{x}\hat{x}^T\right) a_i, \\ &= b^2 - b^2 = 0, \end{aligned}$$

$i = 1, \ldots, m$. We showed that $U[N \setminus P]$ satisfies the first constraint of $(P_{\hat{x}}^{DN})$. Observe that for $j = 1, \ldots, k-p$

$$\begin{aligned} (U[N \setminus P])_{jj} &= U_{j+p,j+p}, \\ &= \hat{X}_{j+p,j+p} - \hat{x}_{j+p}^2, \\ &= \hat{x}_{j+p} - \hat{x}_{j+p}^2, \\ &= w_j - w_j^2, \end{aligned}$$

and thus second constraint of $(P_{\hat{x}}^{DN})$ is satisfied. Since $ww^T + U[N \setminus P] = \hat{X}[N \setminus P] \in \mathcal{N}$ third constraint of $(P_{\hat{x}}^{DN})$ is satisfied. Since $U[N \setminus P] \in \mathcal{PSD}$, last constraint of $(P_{\hat{x}}^{DN})$ is also satisfied. Therefore, we showed that $U[N \setminus P] \in \text{Feas}(P_{\hat{x}}^{DN})$.

Proof of the reverse implication is done by using the same arguments. Therefore, we conclude that for every feasible solution to (3.49) there exists a feasible solution to $(P_{\hat{x}}^{DN})$ and vice versa. By Lemma 3, this implies $\hat{x} \in F_{DN}$ if and only if $(P_{\hat{x}}^{DN})$ is feasible. □

By exploiting the structure of the problem $(P_{\hat{x}}^{DN})$, in the following corollary, we will establish some sufficient conditions that ensure its infeasibility.

Corollary 2. *Let $\hat{x} \in F_{Rel}^{-}$, where F_{Rel}^{-} is defined as in (3.25). Let v_i, $i = 1, \dots, m$ and w be defined as in (3.52) and (3.53), respectively. $(P_{\hat{x}}^{DN})$ is infeasible, i.e., $\hat{x} \notin F_{DN}$, if at least one of the following conditions holds:*

(i) There exists v_i, $i \in \{1, \dots, m\}$, $h \in \{1, \dots, k-p\}$ such that $(v_i)_h \neq 0$ and

$$\begin{aligned} (v_i)_j (v_i)_l &\geq 0, \quad \text{if } w_j w_l = 0, \\ (v_i)_j (v_i)_l &= 0, \quad \text{otherwise} \end{aligned}$$

for all $1 \leq j < l \leq n-p$.

(ii) $\mathrm{Null}(V^T) = 0$, where $V = [v_1 \ v_2 \ \dots \ v_m]$ and $\mathrm{Null}(\cdot)$ denotes the null space.

Proof. Suppose (i) holds. Then, due to third constraint of $(P_{\hat{x}}^{DN})$ observe that $X_{jl} \geq 0$ if $w_j w_l = 0$, $1 \leq j < l \leq n-p$. If we write first constraint for that specific $i \in \{1, \dots, m\}$,

$$v_i^T X v_i = \underbrace{\sum_{j=1}^{n-p} {(v_i)_j}^2 X_{jj}}_{>0} + \sum_{\substack{j \\ w_j w_l > 0}} \sum_{l} \underbrace{(v_i)_j X_{jl} (v_i)_l}_{=0} + \sum_{\substack{j \\ w_j w_l = 0}} \sum_{l} \underbrace{(v_i)_j X_{jl} (v_i)_l}_{\geq 0} > 0$$

which implies that first constraint is violated. Therefore, $(P_{\hat{x}}^{DN})$ is feasible.

Suppose (ii) holds. For a contradiction, suppose there exists $X \in \mathrm{Feas}(P_{\hat{x}}^{DN})$. Since $\hat{x} \in \mathrm{Feas}(\mathrm{Rel}(\mathrm{MBP})) \setminus \mathrm{Conv}(\mathrm{Feas}(\mathrm{MBP}))$, observe that $X \neq 0$. Since $X \in \mathcal{PSD}^{(n-p)}$, then $X = LL^T$. Then

$$\begin{aligned} {v_i}^T X v_i = 0 \quad &\Longrightarrow \quad ({v_i}^T L)^2 = 0 \\ &\Longrightarrow \quad {v_i}^T L = 0 \\ &\Longrightarrow \quad \text{All columns of } L \text{ are orthogonal to } v_i \end{aligned}$$

for all $i = 1, \dots, m$. Since $X \neq 0$, $L \neq 0$ as well. This contradicts with the fact that $\text{Null}(V^T) = 0$. □

Note that Corollary 2 is a technical result, but later on, it will be useful for us in the proof of an important result (see Proposition 10) for the doubly nonnegative relaxation of the 0-1 knapsack problem in Chapter 4.

3.5 Extensions to Mixed Binary Quadratic Programs

In this section, we consider the *mixed binary quadratic program* (MBQP), which is given by

$$\begin{array}{llll} \text{(MBQP)} & \nu^Q := & \min & x^T Q x + c^T x \\ & & \text{s.t.} & {a_i}^T x = b_i, \quad i = 1, \dots, m, \\ & & & x \geq 0, \\ & & & x_j \in \{0,1\}, \quad j \in B, \end{array} \tag{3.54}$$

where $x \in \mathbb{R}^n$ is the decision variable; $Q \in \mathcal{S}^n$, $a_i \in \mathbb{R}^n$, $b \in \mathbb{R}^m$ and $B \subseteq \{1, \dots, n\}$ are the problem parameters. Note that (MBP) is a special case of (MBQP) with $Q = 0$. Under Burer's key assumption [18], (MBQP) can be equivalently formulated as the following completely positive optimization problem:

$$\begin{array}{llll} \text{(MBQP-CP)} & \nu^Q := & \min & \langle Q, X \rangle + c^T x \\ & & \text{s.t.} & {a_i}^T x = b_i, \quad i = 1, \dots, m, \\ & & & {a_i}^T X a_i = {b_i}^2, \quad i = 1, \dots, m, \\ & & & x_j = X_{jj}, \quad j \in B, \\ & & & \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \in \mathcal{CP}, \end{array} \tag{3.55}$$

Note that the only difference of (MBQP-CP) from (MBP-CP) is its objective function. Although its objective function is still linear, now we have an additional term $\langle Q, X \rangle$. Both (MBQP) and (MBQP-CP) are NP-hard optimization problems. Similar to LP relaxation of (MBP), if we relax the binary variables of (MBQP) so that $0 \leq x_j \leq 1$, $j \in B$, we get

$$\text{Rel(MBQP)} \quad \ell_{QP} := \min \quad x^T Q x + c^T x \quad \text{s.t.} \quad {a_i}^T x = b_i, \quad i = 1, \ldots, m, \quad x \geq 0. \tag{3.56}$$

Recall that we do not need $x_j \leq 1$, since it is already implied by $a_i^T x = b_i$, $i = 1, \ldots, m$, due to the key assumption. However, unlike Rel(MBP), Rel(MBQP) is not an LP and it is still an NP-hard problem in general (unless Q is positive or negative semidefinite). If we write the lower bounds for (MBQP-CP) (or (MBQP)) arising from the previously discussed outer approximations,

$$\ell_{sp}^Q := \min\{\langle Q, X\rangle + c^T x : (x, X) \in \text{Feas(SPR)}\},$$
$$\ell_r^Q := \min\{\langle Q, X\rangle + c^T x : (x, X) \in \text{Feas}(\text{Out})_r\}, \quad r \in \mathbb{N},$$
$$\ell_{DN}^Q := \min\{\langle Q, X\rangle + c^T x : (x, X) \in \text{Feas(DN)}\}.$$

Recall that $(\text{Out})_r$ and (DN) are special cases of (SPR). F_{sp}, F_r and F_{DN} remain the same as defined in (3.6), (3.12) and (3.48), respectively. Now, consider Lemma 2. Note that $F_{sp} \subseteq \text{Feas(Rel(MBQP))}$ still holds. However, unlike the previous result in Lemma 2, this does not imply $\ell_{sp}^Q \leq \ell_{QP}$ in general. This is because objective functions of Rel(MBQP) and (SPR) are now different: Rel(MBQP) has $x^T Q x + c^T x$, whereas (SPR) has $\langle Q, X\rangle + c^T x$ as its objective function.

In this section, we investigate the lower bounds arising from the outer approximations of (MBQP-CP). We will give characterizations for their unboundednes. We show that unlike our results on (MBP), those lower bounds are incomparable to that of Rel(MBQP), in general. However, we achieve to establish a sufficient condition, under which any (SPR) gives a lower bound which is at least as tight as the lower bound provided by Rel(MBQP).

3.5.1 Characterizations for the Unboundedness

In this section, we present characterizations for the unboundedness of outer approximations. We also give examples that indicate different possible cases for when the unbondedness of outer approximations and that of Rel(MBQP) is considered together. First, let us characterize the unboundedness of (MBQP).

Proposition 4. *Suppose* Feas(MBQP) *is nonempty.* (MBQP) *is unbounded if and only if at least one of the conditions given below is satisfied:*

(i) There exists $d \in \mathbb{R}^n_+$ *such that* $d^T Qd < 0$, $a_i^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

(ii) There exists $x \in \text{Feas(MBQP)}$ *and* $d \in \mathbb{R}^n_+$ *such that* $d^T Qd = 0$, $(2Qx+c)^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

Proof. Suppose Feas(MBQP) is nonempty. If (MBQP) is unbounded, then there exists $x \in \text{Feas(MBQP)}$ and a direction $d \in \mathbb{R}^n$ such that

$$(x + \lambda d) \in \text{Feas(MBQP)} \tag{3.57}$$

for all $\lambda \geq 0$. Now, let us define the following function:

$$f(\lambda) := (x + \lambda d)^T Q(x + \lambda d) + c^T (x + \lambda d), \quad \lambda \geq 0$$

Then, due to unboundedness of (MBQP), as $\lambda \to +\infty$, $f(\lambda) \to -\infty$. Then, since $f(\lambda)$ is a polynomial function whose degree is at most 2, then either

$$f''(\lambda) < 0 \tag{3.58}$$

or

$$f''(\lambda) = 0 \text{ and } f'(\lambda) < 0. \tag{3.59}$$

for all $\lambda \in \mathbb{R}$. (3.58) implies $d^T Qd < 0$, whereas (3.59) implies $d^T Qd = 0$ and $(2Qx + c)^T d < 0$. Together, (3.57) and (3.58) imply (i), whereas (3.57) and (3.59) imply (ii).

Converse argument is trivial. Therefore, we conclude that (MBQP) is unbounded if and only if (i) or (ii) holds. □

Now, we give the characterization for the unboundedness of Rel(MBQP), which is very similar to that of (MBQP) with a minor difference: item (ii) in Proposition 4 requires the existence of an $x \in \text{Feas(MBQP)}$, whereas item (ii) in the following proposition requires the existence of an $x \in \text{Feas(Rel(MBQP))}$.

Proposition 5. *Suppose* Feas(Rel(MBQP)) *is nonempty.* Rel(MBQP) *is unbounded if and only if at least one of the conditions given below is satisfied:*

(i) There exists $d \in \mathbb{R}^n_+$ *such that* $d^TQd < 0$, $a_i^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

(ii) There exists $x \in \text{Feas(Rel(MBQP))}$ *and* $d \in \mathbb{R}^n_+$ *such that* $d^TQd = 0$, $(2Qx + c)^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

Proof. Proof is done with the same arguments used in Proposition 4. □

Note that items (i) in Propositions 4 and 5 are the same, whereas there is a minor difference in items (ii) as discussed. By exploiting that difference, we later on show in Example 7 that there are some instances for which (MBQP) is bounded, but Rel(MBQP) is unbounded.

We now give two sufficient conditions for the unboundedness of a general (SPR) in the following proposition.

Proposition 6. *Suppose* (SPR) *is defined over the cone* $\mathcal{K} \supseteq \mathcal{CP}$ *and* Feas(SPR) *is nonempty.* (SPR) *is unbounded if at least one of the conditions given below is satisfied:*

(a) The recession cone of Feas(SPR), *i.e.,*

$$\mathcal{L}_\infty := \left\{ \begin{bmatrix} 0 & d^T \\ d & D \end{bmatrix} \in \mathcal{K} : \begin{array}{ll} a_i^T d = 0, & i = 1, \ldots, m \\ a_i^T D a_i = 0, & i = 1, \ldots, m \\ d_j = D_{jj} = 0, & j \in B \end{array} \right\}$$

contains a pair (d, D) *such that* $\langle Q, D\rangle + c^T d < 0$,

(b) There exists $x \in F_{sp}$ *and* $d \in \mathbb{R}^n_+$ *such that* $d^T Q d = 0$, $(2Qx + c)^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

Proof. Suppose item (a) holds. Let $(\hat{d}, \hat{D}) \in \mathcal{L}_\infty$ be such $\langle Q, D\rangle + c^T d < 0$. Let $(\hat{x}, \hat{X}) \in$ Feas(SPR). Let $(x_\lambda, X_\lambda) := (\hat{x}, \hat{X}) + \lambda(\hat{d}, \hat{D})$, where $\lambda \in \mathbb{R}$. Observe that $(x_\lambda, X_\lambda) \in$ Feas(SPR) and $\langle Q, X_\lambda\rangle + c^T x_\lambda \to -\infty$ as $\lambda \to \infty$. Suppose (b) holds. Let $\hat{x} \in F_{sp}$ and $d \in \mathbb{R}^n_+$ satisfying the necessities given (b). Then, unboundedness under (b) is shown by a similar argument that we used for (a). □

Note that Proposition 6 will be useful for us while establishing our results regarding especially the unboundedness of doubly nonnegative relaxations.

Outer Polyhedral Approximations

We investigate the unboundedness of outer polyhedral approximations due to de Klerk and Pasechnik [22]. Recall that these approximations are sign preserving approximations. Therefore, Proposition 6 applies to them as well. However, since $\mathcal{O}_0 = \mathcal{N}$, we can give the following simple characterization for the unboundedness of $(\text{Out})_0$.

Corollary 3. *Suppose* $\text{Feas}(\text{Out})_0$ *is nonempty.* $(\text{Out})_0$ *is unbounded if and only if at least one of the conditions given below is satisfied:*

(i) There exists $d \in \mathbb{R}^n_+$ *such that* $c^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$, *and* $d[B] = 0$.

(ii) There exists $D \in \mathcal{N}$ *such that* $\langle D, Q\rangle < 0$, ${a_i}^T D a_i = 0$, $i = 1, \ldots, m$, $D_{jj} = 0$, $j \in B$.

Proof. Suppose $(\text{Out})_0$ is unbounded. Then either (i) or (ii) must hold trivially, since $(\text{Out})_0$ is an LP problem. Reverse implication is also trivial. □

We now establish a relationship between the unboundedness of Rel(MBQP) and $(\text{Out})_0$ in the following theorem.

Theorem 6. *Suppose* Feas(MBQP) *is nonempty. If* Rel(MBQP) *is unbounded, then* $(\text{Out})_0$ *is also unbounded.*

Proof. Suppose Rel(MBQP) is unbounded. Then, either (i) or (ii) in Proposition 5 holds. Suppose (i) holds. Then, setting $D = dd^T$ observe that item (ii) in Corollary 3 holds. Otherwise suppose item (ii) in Proposition 5 holds. Then, there exists $x \in$ Feas(Rel(MBQP)) and $d \in \mathbb{R}^n_+$ such that $d^T Q d = 0$, $(2Qx + c)^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$ and $d[B] = 0$. $(2Qx + c)^T d < 0$ implies either $c^T d < 0$ or $x^T Q d = \langle Q, xd^T \rangle < 0$ holds. If $c^T d < 0$, then item (i) in Corollary 3 holds. Otherwise, setting $D = xd^T + dx^T$, observe that item (ii) in Corollary 3 holds. This completes the proof. □

Now, we will device an example, where (MBQP) is bounded, but Rel(MBQP) and $(\text{Out})_r$ are unbounded. However, since item (i) is common in Propositions 4 and 5, we first have to make sure that it does not hold. Let $C := \{1, \ldots, n\} \setminus B$. Observe that positive semidefiniteness of $Q[C]$ suffices to ensure $d^T Q d \geq 0$ since $d[B] = 0$. Consider the following example.

Example 7.

$$Q = \begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 1.4 & -1 & 0 \\ -1 & -1 & 1.4 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$c = 0,$$

$$x_1 + x_4 = 0.7,$$

$$x_2, x_3, x_4 \geq 0,$$

$$x_1 \in \{0, 1\}.$$

If we consider (MBQP)*, observe that x_1 must be equal to 0. Then, objective turns into "*min $(x_2 - x_3)^2 + 0.4x_2^2 + 0.4x_3^2$*" with $\nu^Q = 0$ obviously. However, if we consider* Rel(MBQP)*, setting initial point $x^T = \begin{bmatrix} 0.5 & 1 & 1 & 0.2 \end{bmatrix} \in$* Feas(Rel(MBQP)) *and direction $d^T = \begin{bmatrix} 0 & 1 & 1 & 0 \end{bmatrix}$, we can decrease objective function as much as we want while staying in the feasible region, i.e., $\ell_{QP} = -\infty$. Lastly, for $(\text{Out})_0$, setting $D_{12} = D_{21} = 1$ and all other values of D equal to 0, observe that (ii) in* Corollary 3 *is realized. Therefore, $(\text{Out})_0$ is also unbounded, i.e., $\ell_0^Q = -\infty$.*

Now, we will device another example, where (MBQP) and Rel(MBQP) are bounded, but $(\text{Out})_r$ is unbounded. To do that, we first have to make sure both (*i*) and (*ii*) in Proposition 5 do not hold. Observe that positive definiteness of Q suffices to ensure it. Consider the following example.

Example 8.

$$Q = \begin{bmatrix} 6 & -1.7 & -2.5 & 2.8 \\ -1.7 & 7.2 & 0.3 & 2 \\ -2.5 & 0.3 & 1.3 & -0.8 \\ 2.8 & 2 & -0.8 & 3.9 \end{bmatrix}$$

$$c = 0,$$

$$x_1 + x_4 = 0.7,$$

$$x_2, x_3, x_4 \geq 0,$$

$$x_1 \in \{0, 1\}.$$

Observe that Q is positive definite and thus both (MBQP) *and* Rel(MBQP) *are bounded. Optimal value and optimal solution of* (MBQP) *are $\nu^Q \approx 1.67$, $x^{*T} \approx \begin{bmatrix} 0 & 0 & 0.43 & 0.7 \end{bmatrix}$, respectively. Optimal value and optimal solution of* Rel(MBQP) *are $\ell_{QP} \approx 0.498$, $x^{*T} \approx \begin{bmatrix} 0.7 & 0.11 & 1.32 & 0 \end{bmatrix}$, respectively. Lastly, as in* Example 7, *setting $D_{12} = D_{21} = 1$ and all other values of D equal to 0, observe that (ii) in* Corollary 3 *is realized. Therefore, $(\mathrm{Out})_0$ is unbounded, i.e., $\ell_0^Q = -\infty$.*

So far we simplified the characterization for the unboundedness of $(\mathrm{Out})_0$. By Theorem 6, we showed that if Rel(MBQP) is unbounded, then $(\mathrm{Out})_0$ must be unbounded. We also exploited the conditions given in Proposition 5 and Corollary 3 to devise Examples 7 and 8.

Note that Proposition 6 also applies to higher levels of outer approximations. If the instance given in Example 7 is solved for higher levels of $r \in \mathbb{N}$, then it turns out that $\ell_r^Q = -\infty$ for $r = 0, 1, \ldots, 15$, whereas $(\mathrm{Out})_{16}$ is bounded with $\ell_{16}^Q \approx -9.32$. Similarly, if the instance given in Example 8 is solved for higher levels, then $\ell_r^Q = -\infty$ for $r = 0, 1, \ldots, 4$; whereas $(\mathrm{Out})_5$ is bounded with $\ell_5 \approx -6.83$, though it is still much worse lower bound than $\ell_{QP} \approx 0.498$.

Doubly Nonnegative Relaxations

Recession cone of Feas(DN) can be given as

$$\left\{ \begin{bmatrix} 0 & 0^T \\ 0 & D \end{bmatrix} \in \mathcal{DN} : \begin{array}{ll} a_i^T D a_i = 0, & i = 1, \ldots, m \\ D_{jj} = 0, & j \in B \end{array} \right\}.$$

Therefore, the following corollary directly follows from Proposition 6.

Corollary 4. *Suppose* Feas(DN) *is nonempty.* (DN) *is unbounded if at least one of the conditions given below is satisfied:*

(i) There exists $D \in \mathcal{DN}$ *such that* $\langle D, Q \rangle < 0$, ${a_i}^T D a_i = 0$, $i = 1, \ldots, m$, $D_{jj} = 0$, $j \in B$.

(ii) There exists $x \in F_{DN}$ *and* $d \in \mathbb{R}^n_+$ *such that* $d^T Q d = 0$, $(2Qx + c)^T d < 0$, ${a_i}^T d = 0$, $i = 1, \ldots, m$ *and* $d[B] = 0$.

Following will constitute an example to the case where (MBQP) and (DN) are bounded, but Rel(MBQP) is unbounded.

Example 9. *Consider the instance given in* Example 7. *We already know that* Rel(MBQP) *is unbounded for that instance. Since* $n \leq 4$*, by Diananda's result [23]* $\mathcal{DN} = \mathcal{CP}$*, which implies that* $\nu^Q = \ell^Q_{DN} = 0$.

Now, we will give an example, for which (MBQP) is bounded, but both (DN) and Rel(MBQP) are unbounded. To do that, we exploit the item (*ii*) in Proposition 5 and item (*i*) in Corollary 4. Building such an example is not as easy as the previous example. Due to (*i*) in Corollary 4, we need a $D \in \mathcal{DN}$ and $Q \in \mathcal{S}^n$ such that $\langle Q, D \rangle < 0$, which implies $Q \notin \mathcal{SPN}$. Also, item (*i*) in Proposition 4 needs to be violated, because otherwise (MBQP) becomes unbounded. To ensure that, we will pick a matrix $Q \in \mathcal{COP}$. Therefore, we need $Q \in \mathcal{COP} \setminus \mathcal{SPN}$. As given in Example 10, Q is not positive definite or negative semidefinite. Therefore, solving (MBQP) and Rel(MBQP) for such an instance is a task where solvers are having difficulties. Nevertheless, we will luckily be able to derive the optimal values theoretically. While generating the matrix Q, we will utilize the following Horn matrix

$$H := \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}. \tag{3.60}$$

This matrix was first established by Horn [35] and he showed that $H \in \mathcal{COP} \setminus \mathcal{SPN}$. Now, consider the following matrix

$$Z := \begin{bmatrix} 7 & 4 & 0 & 0 & 4 \\ 4 & 7 & 4 & 0 & 0 \\ 0 & 4 & 7 & 4 & 0 \\ 0 & 0 & 4 & 7 & 4 \\ 4 & 0 & 0 & 4 & 7 \end{bmatrix} \tag{3.61}$$

Note that $Z \in \mathcal{DN}^5$, but $Z \notin \mathcal{CP}^5$, since $\langle Z, H \rangle = -5 < 0$. Therefore $Z \in \mathcal{DN} \setminus \mathcal{CP}$.

Now by utilizing the matrices H and Z, we construct an example in which (MBQP) is bounded, but both (DN) and Rel(MBQP) are unbounded.

Example 10. *Consider the following* (MBQP) *instance.*

$$Q = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 1 & 1 & -1 & 0 \\ -1 & -1 & 1 & -1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 1 & 1 & -1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad c = 0,$$

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$b = 0.7,$$

$$x \geq 0,$$

$$x_1 \in \{0, 1\}.$$

Define $\alpha := \{2, \ldots, 7\}$, $\beta := \{2, \ldots, 6\}$. *Observe that* $Q[\beta] = H$, *where* H *is defined in* (3.60). *Observe that* $x_1 = 0$ *for all* $x \in \text{Feas(MBQP)}$. *Then, if we consider the objective function of* (MBQP),

$$x^T Q x = x[\alpha]^T Q[\alpha] x[\alpha]$$

for all $x \in \text{Feas(MBQP)}$. *Also, since* 7^{th} *column and row of* Q *is all 0*

$$x[\alpha]^T Q[\alpha] x[\alpha] = x[\beta]^T Q[\beta] x[\beta] = x[\beta]^T H x[\beta],$$

for all $x \in \text{Feas(MBQP)}$. *Since* $x[\beta] \geq 0$ *and* $H \in \mathcal{COP}$, *we have* $x^T Q x = x[\beta]^T Q[\beta] x[\beta] \geq 0$ *for all* $x \in \text{Feas(MBQP)}$. *Therefore* $\nu^Q \geq 0$. *Observe that* $\hat{x} := \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0.7 \end{bmatrix} \in \text{Feas(MBQP)}$ *and* $\hat{x}^T Q \hat{x} = 0$. *Therefore, we conclude that* $\nu^Q = 0$.

Consider Rel(MBQP). *Let* $\bar{x} := \begin{bmatrix} 0.5 & 1 & 1 & 0 & 0 & 0 & 0.2 \end{bmatrix} \in \text{Feas(Rel(MBQP))}$ *and* $d := \begin{bmatrix} 0 & 0.5 & 0.5 & 0 & 0 & 0 & 0 \end{bmatrix}$. *Observe that* $d \geq 0$, $d_1 = 0$, $d^T Q d = 0$ *and*

$(Qx+c)^T d = -0.5 < 0$. *Therefore, by* Proposition 5, *starting from point* $\bar{x}$ *and going through direction* d, *we can decrease the objective function as much as we want while staying in the feasible region. Hence,* $\ell_{QP} = -\infty$.

When we consider (DN), *let*

$$D = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7 & 4 & 0 & 0 & 4 & 0 \\ 0 & 4 & 7 & 4 & 0 & 0 & 0 \\ 0 & 4 & 7 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 7 & 4 & 0 \\ 0 & 4 & 0 & 0 & 4 & 7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Observe that $D[\beta] = Z$, *which is defined in* (3.61). *Therefore* $\langle Q, D\rangle = \langle Q[\beta], D[\beta]\rangle = \langle H, Z\rangle = -5 < 0$. *Also,* $D \in \mathcal{DN}$ *and* ${a_1}^T D a_1 = 0$. *Therefore, by* Proposition 4, *we conclude that* $\ell_{DN}^{Q} = -\infty$.

By modifying Example 10 slightly, we will be able to create an example in which (MBQP) and Rel(MBQP) is bounded, but (DN) is unbounded.

Example 11. *Consider the following* (MBQP) *instance.*

$$Q = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 1 & 1 & -1 & 0 \\ -1 & -1 & 1 & -1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 1 & 1 & -1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad c = 0,$$

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$b^T = \begin{bmatrix} 0.7 & 0 \end{bmatrix},$$

$$x \geq 0,$$

$$x_1 \in \{0, 1\}.$$

Observe that feasible region of this example is the same as that of Example 10*. Therefore* $\nu^Q = 0$*. Also, note that for this instance* Feas(Rel(MBQP)) = Feas(MBQP)*, which implies that* $\ell_{QP} = 0$*. Now consider* D *given in* Example 10*. Observe that* ${a_2}^T D a_2 = 0$ *also holds. Therefore,* $\ell^Q_{DN} = -\infty$*.*

3.5.2 Incomparability of Lower Bounds

In this section, we show that, unlike (MBP), lower bounds arising from the outer approximations of (MBQP-CP) is incomparable with the lower bound provided by Rel(MBQP). As illustrated in Example 8, there exists an (MBQP) instance such that $\ell_{QP} > \ell^Q_0$. Following example illustrates that there also exists an (MBQP) instance such that $\ell^Q_0 > \ell_{QP}$.

Example 12. *Consider the following instance of* (MBQP)*.*

$$Q = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 2 \end{bmatrix}$$

$$c^T = [-1 \ -1 \ 0],$$

$$A = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix},$$

$$b = 1,$$

$$x_1, x_2 \in \{0, 1\},$$

$$x_3 \geq 0.$$

Optimal values and optimal solutions of (MBQP), Rel(MBQP) *and* $(\text{Out})_0$ *are respectively as follows:*

$$\nu^Q = 2, \quad x^{*T} = [0 \ 0 \ 1]$$

$$\ell_{QP} = 1.5, \quad {x^*_{bin}}^T = [0.5 \ 0.5 \ 0]$$

$$\ell_0^Q = 2, \quad x_0^{*T} = [0 \ 0 \ 1], \qquad X_0^* = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Therefore, for this instance we have $\ell_0^Q > \ell_{QP}$*.*

Recall that $\ell_0 \geq \ell_{LP}$ always holds for (MBP) instances. However, by Examples 8 and 12, the similar result does not necessarily apply to (MBQP) problem. Therefore, when the considered problem is (MBQP), we conclude that lower bounds arising from Rel(MBQP) and $(\text{Out})_0$ are incomparable in general. As discussed in the previous section, by Examples 7 and 8, incomparability between the optimal values of $(\text{Out})_r$ and Rel(MBQP) still continues to the higher levels of $r \in \mathbb{N}$ in general. By Examples 9 and 11, it turns out that the optimal values of (DN) and Rel(MBQP) are also incomparable in general, whereas $\ell_{DN} \geq \ell_{LP}$ always holds when the considered problem is (MBP). Therefore, previously established relationships between the lower bounds of (MBP) clearly do not extend to (MBQP) in general.

3.5.3 Sufficient Conditions for Comparability

After showing that our results on (MBP) do not extend to (MBQP), in this section, we give sufficient conditions that ensure lower bounds arising from outer approximations are comparable to the lower bound provided by Rel(MBQP). In the next proposition, we show that, based on the optimal solutions of (SPR), we can give a sufficient condition that ensures $\ell_{sp}^Q \geq \ell_{QP}$.

Proposition 7. *Consider an instance of* (MBQP). *Suppose there exists an optimal solution* (x^*, X^*) *for* (SPR) *such that*

$$\left\langle Q, X^* - x^*(x^*)^T \right\rangle \geq 0. \tag{3.62}$$

Then $\ell_{sp}^Q \geq \ell_{QP}$.

Proof. We know that $\ell_{sp}^Q = \langle Q, X^* \rangle + c^T x^*$. Since $x^* \in F_{sp}$, by Lemma 2, $x^* \in$ Feas(Rel(MBQP)). This implies the following relationship:

$$\ell_{sp}^Q \geq x^{*T} Q x^* + c^T x^* \geq \ell_{QP}.$$

□

Remark 4. *Consider* Example 12. *Observe that* Q *satisfies the condition* (3.62) *given in* Proposition 7. *Therefore, in* Example 12, $\ell_{sp}^Q \geq \ell_{QP}$ *is already implied by* Proposition 7.

In Proposition 7, we gave a sufficient condition that ensures $\ell_{sp}^Q \geq \ell_{QP}$. Recall that (MBP) encompasses all instances of (MBQP) with $Q = 0$. Hence, when the considered instance belongs to (MBP), (3.62) is already satisfied. Therefore, observe that the result $\ell_{sp} \geq \ell_{LP}$ given by Lemma 2 is also implied by Proposition 7.

Following corollary directly follows from Proposition 7 to ensure that (SPR) gives a strictly better lower bound than Rel(MBQP), i.e., $\ell_{sp}^{Q} > \ell_{QP}$.

Corollary 5. *Given an instance of* (MBQP)*, suppose there exists an optimal solution* (x^*, X^*) *for* (SPR) *such that*

$$\left\langle Q, X^* - x^*(x^*)^T \right\rangle > 0. \tag{3.63}$$

Then $\ell_{sp}^{Q} > \ell_{QP}$*.*

Remark 5. *Unfortunately,* Corollary 5 *does not admit an equivalence, i.e., it is possible that* $\ell_{sp}^{Q} > \ell_{QP}$ *can still hold, although* (3.63) *does not hold. Observe that in* Example 12*,* (3.63) *is violated. However,* $\ell_{0}^{Q} > \ell_{QP}$ *still holds for* Example 12*.*

Proposition 7 and Corollary 5 assume that optimal solutions of (SPR) are already achieved. This is a reasonable assumption, since, if (SPR) has a unique optimal solution and a tractable cone in its conic constraint, then the unique optimal solution can be obtained in polynomial-time with respect to problem size. On the other hand, if (SPR) has infinitely many optimal solutions, then identifying a solution that satisfies these conditions can be a difficult task.

Hypothesis of Proposition 7 is dependent on identifying the optimal solutions of (SPR). However, in the next corollary, by exploiting (3.62) in Proposition 7, we achieve to establish a result that is free of that dependency for the case of (DN).

Corollary 6. *Consider an instance of* (MBQP)*. Suppose* Q *is of the form*

$$Q = \sum_{i=1}^{m} \lambda_i a_i a_i^T + D + R, \tag{3.64}$$

such that:

(i) $\lambda_i \in \mathbb{R}$*,* $i = 1, \ldots, m$*.*

(ii) $D \in \mathcal{N}$ *is a diagonal matrix with* $D_{jj} \geq 0$ *for* $j \in B$ *and* $D_{jj} = 0$ *for* $j \in \{1, \ldots, n\} \setminus B$*.*

(iii) $R \in \mathcal{PSD}$.

Then $\ell_{DN}^{Q} \geq \ell_{QP}$.

Proof. Let (x^*, X^*) be an optimal solution of (DN). Observe that $X^* - x^*(x^*)^T \in \mathcal{PSD}$. We will show that (3.62) holds. It can be shown as follows:

$$\begin{aligned}
\left\langle Q, X^* - x^*(x^*)^T \right\rangle &= \left\langle \sum_{i=1}^{m} \lambda_i a_i a_i^T + D + R,\ X^* - x^*(x^*)^T \right\rangle \\
&= \left\langle D, X^* - x^*(x^*)^T \right\rangle + \left\langle R, X^* - x^*(x^*)^T \right\rangle \\
&= \sum_{j \in B} \underbrace{D_{jj}}_{\geq 0} \underbrace{\left(X_{jj}^* - (x_j^*)^2\right)}_{\geq 0} + \underbrace{\left\langle R, X^* - x^*(x^*)^T \right\rangle}_{\geq 0} \\
&\geq 0.
\end{aligned}$$

Therefore, by Proposition 7, we conclude that $\ell_{DN}^{Q} \geq \ell_{QP}$. □

Although ℓ_{DN}^{Q} and ℓ_{QP} are incomparable in general for (MBQP), there are some special cases of (MBQP), to which Corollary 6 apply. We already discussed that (MBP) is one of those special cases. Another special case is the *maximum cut* (MAX-CUT) problem. The objective of (MAX-CUT) is to partition the set of vertices of a graph into two subsets, such that the total weight of the edges having one endpoint in each of the subsets is maximum. This problem is known to be NP-complete [30, 45] and it can be formulated as an instance of (MBQP) with $Q \in \mathcal{PSD}$ and $B = \{1, \ldots, n\}$. Since $Q \in \mathcal{PSD}$, it can be written of the form (3.64) with $(\lambda, D, R) = (0, 0, Q)$. Therefore, $\ell_{DN}^{Q} \geq \ell_{QP}$ holds for (MAX-CUT) problem. For a detailed survey of (MAX-CUT), reader is referred to [77].

3.6 Conclusion

We defined the sign preserving outer approximation which is a more general definition that covers other outer approximations of (MBP-CP). We showed that outer approximations are unbounded if and only if the original problem is unbounded. We compared the lower bounds arising from outer approximations with the lower bound provided by the LP relaxation of (MBP). We established that $\ell_{sp} \geq \ell_{LP}$ always holds for an outer approximation of (MBP-CP) in the class of (SPR). We also gave a characterization to check the equality of the sets F_{sp} and Feas(Rel(MBP)). Note that this characterization is based on enumerating the extreme points of Feas(Rel(MBP)). Therefore, it may not work in polynomial-time with respect to problem size.

For outer polyhedral approximations, we gave a sufficient condition that works in polynomial-time to check the equality between F_0 and Feas(Rel(MBP)). For higher levels of $r \in \mathbb{N}$, given $x \in F^{-}_{Rel}$, we gave a sufficient condition which ensures that $x \in F_r$ holds until at least a certain level $r \in \mathbb{N}$. We also gave a necessary condition for $x \in F_r$, $r \in \mathbb{N}$.

As for the doubly nonnegative relaxations, we have shown that the problem $P_{\hat{x}}$ defined in Lemma 3 can be reduced to a smaller problem. Given $x \in F_{DN}$, by exploiting the structure of our reduced problem, we gave sufficient conditions, under which $x \notin F_{DN}$.

We then investigated the extensions of our results to the mixed binary quadratic programs. We gave the characterizations for the unboundedness of continuous relaxation of (MBQP) and for the unboundedness of outer approximations within our scope. We showed that if Rel(MBQP) is unbounded, then $(\text{Out})_0$ must be unbounded as well. Other than that, we gave an example for the case, in which Rel(MBQP) is bounded, but $(\text{Out})_0$ is unbounded.

As for the doubly nonnegative relaxations, we showed by examples that there is no relationship between the unboundedness of Rel(MBQP) and (DN). We next showed that, unlike (MBP), lower bounds arising from the completely positive formulation of (MBQP) are not comparable to the lower bound given by Rel(MBQP) in general. However, we gave a sufficient condition in Proposition 7, under which $\ell^{Q}_{sp} \geq \ell_{QP}$ is assured. It turns out that Proposition 7 actually serves as an extension to (MBP) case. We also gave a sufficient condition in Corollary 5 for outer approximations to provide strictly better lower bounds than that of Rel(MBQP).

Finally, for the doubly nonnegative relaxations, to ensure that $\ell_{DN}^{Q} \geq \ell_{QP}$, we showed in Corollary 6 that we can get rid of the necessity of enumerating over optimal solutions by strengthening the sufficient condition of Proposition 7. We also discussed the fact that Corollary 6 applies to the doubly nonnegative relaxations of (MAX-CUT) problem and therefore $\ell_{DN}^{Q} \geq \ell_{QP}$ always holds for it.

Chapter 4

OUTER APPROXIMATIONS OF THE 0-1 KNAPSACK PROBLEM

4.1 Introduction

In this chapter, we will investigate the outer approximations of the completely positive formulation of the 0-1 knapsack problem. The 0-1 knapsack problem is a well-known and extensively studied problem in the literature (see, e.g., [64, 51, 83, 55, 72]). Given a set of items $N := \{1, \ldots, n\}$, in which each item has a weight $a_i \in \mathbb{R}_+$ and value $c_i \in \mathbb{R}_+$, $i = 1, \ldots, n$, along with a knapsack capacity $b \in \mathbb{R}_+$; the objective of this problem is to find $N' \subseteq N$ such that the total weight of the items in N' does not exceed the capacity b, whereas the total value of them is as large as possible. Formally, it can be given as

$$
\begin{array}{llll}
\text{(KP)} & \nu := & \max & c^T x \\
 & & \text{s.t} & a^T x \leq b, \\
 & & & x_i \in \{0, 1\} \quad i = 1, \ldots, n,
\end{array}
$$

where $x \in \mathbb{R}^n$ is the decision variable, $c,\ a \in \mathbb{R}^n_+$ and $b \in \mathbb{R}_+$ are the problem parameters. If there exists a a_i, $i \in \{1, \ldots, n\}$, such that $a_i > b$, then clearly x_i will be equal to 0. Therefore, throughout this chapter, without loss of generality we will assume that $a_i \leq b$, for all $i = 1, \ldots, n$.

Despite its simple representation, it is well-known that (KP) is NP-hard [52, 30]. There are many solution approaches proposed to solve (KP) in the literature. Among them, dynamic programming [3], branch-and-bound [64] and hybridization of both approaches [76, 62, 75, 63] are the most notable ones. Aside from these specific solution efforts, it can also be solved by brute force via enumeration of all 2^n possible subsets of N.

Note that with a little modification (KP) can be put into the form of (MBP). First write the inequality constraint as equality. Secondly, since (KP) does not necessarily satisfy Burer's *key assumption* [18], add the constraints $x_i + s_i = 1$, $i = 1, \dots, n$. After these modifications, we get

$$
\begin{array}{llll}
(\mathrm{KP})_{aug} & \nu := & \max & c^T x \\
 & & \text{s.t} & a^T x + \theta = b, \\
 & & & x_i + s_i = 1, \quad i = 1, \dots, n, \\
 & & & \theta \geq 0, \\
 & & & x_i \in \{0, 1\} \quad i = 1, \dots, n,
\end{array}
$$

where $s \in \mathbb{R}^n$ and θ are slack variables. Note that $(\mathrm{KP})_{aug}$ is a special case of (MBP) with $m = n + 1$, and $B = \{1, \dots, n\}$. Therefore, the reader should take a note that all the given results that apply to (MBP) in Chapter 3 also apply to the 0-1 knapsack problem. (KP) can therefore be equivalently formulated as the following instance of completely positive optimization problem [18]:

$$
\begin{array}{llll}
(\text{KP-CP})^1 & \nu = & \max & c^T x \\
 & & \text{s.t} & a^T x + \theta = b, \\
 & & & a^T x + 2a^T v + \omega = b^2, \\
 & & & x_i + s_i = 1, \quad i = 1, \dots, n \\
 & & & X_{ii} + 2R_{ii} + S_{ii} = 1, \quad i = 1, \dots, n \\
 & & & x_i = X_{ii}, \quad i = 1, \dots, n \\
 & & & \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \mathcal{CP},
\end{array}
$$

where $X,\ S \in \mathcal{S}^n,\ R \in \mathbb{R}^{n\times n},\ x,\ s,\ v,\ y \in \mathbb{R}^n$ and $\theta, \omega \in \mathbb{R}$ are decision variables, $c,\ a \in \mathbb{R}^n_+$ and $b \in \mathbb{R}_+$ are the problem parameters.

We will also present another copositive reformulation of (KP). In $(\text{KP})_{aug}$, observe that although $s \in \mathbb{R}^n$ is continuous, it will have binary entries due to the binary restriction on the entries of x and second constraint. Therefore, adding binary constraints $s_i \in \{0,1\}$ to $(\text{KP})_{aug}$ will be redundant, but it gives rise to another copositive reformulation that yields tighter outer approximations than $(\text{KP-CP})^1$:

$$
\begin{array}{llll}
(\text{KP-CP})^2 & \nu = & \max & c^T x \\
& & \text{s.t} & a^T x + \theta = b, \\
& & & a^T x + 2a^T v + \omega = b^2, \\
& & & x_i + s_i = 1, \quad i = 1, \ldots, n \\
& & & R_{ii} = 0, \quad i = 1, \ldots, n \\
& & & X_{ii} = x_i, \quad i = 1, \ldots, n \\
& & & S_{ii} = s_i, \quad i = 1, \ldots, n \\
& & & \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \mathcal{CP},
\end{array}
$$

Note that $(\text{KP-CP})^1$ and $(\text{KP-CP})^2$ are exact reformulations of (KP). We will investigate both of these copositive formulations in this chapter.

This chapter is organized as follows: We define our notation and go over the well-known linear programming (LP) relaxation of (KP) in Section 4.2. In comparison with the LP relaxation of (KP), we investigate the feasible regions and optimal values of outer approximations in Section 4.3. We first make our analysis for level 0 and then for higher levels of $r \in \mathbb{N}$. Section 4.4 is devoted to the doubly nonnegative relaxations of (KP-CP). Similar to Section 4.3, we will compare feasible regions and lower bounds arising from these relaxations with those provided by the LP relaxation of (KP). We conclude the chapter by discussing our results in Section 4.5.

4.2 Preliminaries

4.2.1 Notation

$e^n \in \mathbb{R}^n$ will denote the vector of all ones and $0^n \in \mathbb{R}^n$ will denote the vector of all zeros. e_i will denote the standard unit vector whose i^{th} element is equal to 1 and all others are equal to 0. Dimension of e_i will always be clear from the context. We adopt a Matlab-like notation to denote subvectors and submatrices. For instance, given a vector $u \in \mathbb{R}^n$, $u_{1:p} \in \mathbb{R}^p$ denotes the subvector of u indexed by $1, \ldots, p$. Similarly, given $M \in \mathcal{S}^n$, $M_{I,J} \in \mathbb{R}^{|I| \times |J|}$ denotes the submatrix of M whose rows and columns are indexed by I and J, respectively. Diag$(\cdot)$ returns a square diagonal matrix which consists of the entries of a given vector on the main diagonal.

Feas$(\cdot)$ will denote the feasible region of a given problem. Set of extreme points of a given set will be denoted by $\mathcal{E}(\cdot)$. Conv$(\cdot)$ will denote the convex hull of a given set. Given two matrices $X,\ Y \in \mathbb{R}^{m \times n}$, $\langle X, Y \rangle$ will denote the trace inner product, i.e.,

$$\langle X, Y \rangle = \sum_{i=1}^{m} \sum_{j=1}^{n} X_{ij} Y_{ij}.$$

4.2.2 Linear Programming Relaxation of the 0-1 Knapsack

By relaxing the binary restrictions of the variables to $x_i \in [0,1]$, $i = 1, \ldots, n$, linear programming (LP) relaxation of the knapsack problem can be given as

$$\begin{array}{llll} \text{Rel(KP)} & u_{LP} := & \max & c^T x \\ & & \text{s.t} & a^T x \leq b, \\ & & & 0 \leq x_i \leq 1, \quad i = 1, \ldots, n, \end{array}$$

First, we want to point out the special structure of the extreme points of Rel(KP) in the following lemma.

Lemma 7. *An arbitrary extreme point of* Feas(Rel(KP)) *has at most 1 fractional value.*

Proof. For an LP problem, extreme point and basic feasible solution (BFS) are equivalent terms. Hence, if we look at Rel(KP), there are $2n+1$ inequality constraints and n variables. Any non-degenerate BFS should satisfy exactly n constraints as equality.

There are two possible cases: Either first constraint ($a^T x \leq b$) is satisfied as equality or not. If the first constraint is satisfied as equality, then $n-1$ constraints out of $2n$ constraints must be satisfied as equality, which in turn implies that $n-1$ elements of a BFS must be equal to either 0 or 1 and exactly one element must be fractional between 0 and 1.

Now, suppose first constraint is satisfied strictly. Then, obviously, all n elements of a BFS must be equal to either 0 or 1, which implies that BFS does not have a fractional element.

Lastly, if we consider a degenerate BFS, then it satisfy more than n constraints as equality. Based on this fact, observe that all n elements of a degenerate BFS must be equal to either 0 or 1, which again implies that a degenerate BFS does not have a fractional element.

Finally, for all possible cases we showed that an arbitrary $x \in \mathcal{E}(\text{Feas}(\text{Rel}(\text{KP})))$ has at most 1 fractional value. □

After establishing this fact about the extreme points, note that there is a simple and well-known algorithm to solve Rel(KP): First, items can be renumbered without loss of generality, so that

$$\frac{c_1}{a_1} \geq \frac{c_2}{a_2} \geq \ldots \geq \frac{c_n}{a_n}. \tag{4.1}$$

Then, items are placed in the knapsack one by one in this order. This process continues until (a) all of the items are placed in the knapsack or (b) until the items completely fill the knapsack's capacity without disruption, or (c) the remaining capacity of the knapsack is filled in such a way that the next item is to be loaded in a fractional manner [55]. In all three cases, an optimal solution for Rel(KP) is obtained. Note that there may be multiple optimal solutions if some inequalities in (4.1) are achieved as equality. For the cases (a) and (b), an optimal solution of Rel(KP) becomes an optimal solution of (KP) as well. If case (c) occurs, an optimal solution for Rel(KP) can be given as follows:

$$x_i^* = \begin{cases} 1 & i = 1, \ldots, k, \\ \dfrac{b - \sum_{j=1}^{k} a_j}{a_{k+1}} & \text{for } i = k+1, , \\ 0 & \text{otherwise,} \end{cases} \tag{4.2}$$

where $a_{k+1} > 0$ and $k < n$ is such that

$$\sum_{i=1}^{k} a_i < b \quad \text{and} \quad \sum_{i=1}^{k+1} a_i > b, \tag{4.3}$$

and thus x_{k+1}^* becomes the only fractional element of the optimal solution x^*. Given x is an extreme point of Feas(Rel(KP)) with one fractional, without loss of generality (w.l.o.g.), we will always assume that first k elements of x is equal to 1, $(k+1)^{th}$ element is fractional, and the remaining elements are equal to 0.

Following is proven in [55], but for the sake of completeness we will include its proof here.

Lemma 8. *Given a* (KP) *instance,* $\nu \leq u_{LP} < 2\nu$ *holds.*

Proof. If $\nu = u_{LP}$, then assertion follows. Otherwise, if $\nu < u_{LP}$, observe that all optimal solutions of Rel(KP) are of the form (4.2). In this case,

$$u_{LP} = \sum_{i=1}^{k} c_i + c_{k+1} \left(\frac{b - \sum_{j=1}^{k} a_j}{a_{k+1}} \right).$$

Observe that $x = \sum_{i=1}^{k} e_i$ is a feasible solution for (KP), which implies that $\sum_{i=1}^{k} c_i \leq \nu$. Since $a_{k+1} \leq b$, $x = e_{k+1}$ is also a feasible solution for (KP), which implies that $c_{k+1} \leq \nu$. Therefore,

$$u_{LP} = \underbrace{\sum_{i=1}^{k} c_i}_{\leq \nu} + \underbrace{c_{k+1}}_{\leq \nu} \underbrace{\left(\frac{b - \sum_{j=1}^{k} a_j}{a_{k+1}} \right)}_{<1} < 2\nu.$$

□

Remark 6. *Although the second inequality in Lemma 8 is strict, note that there may be instances of* (KP) *for which u_{LP} is infinitesimally close to 2ν. For example consider the following instance*

$$\begin{aligned} \max \quad & x_1 + x_2 \\ \text{s.t.} \quad & x_1 + x_2 \leq 2 - \epsilon, \\ & x_i \in \{0,1\}, \quad i = 1,2, \end{aligned}$$

where $\epsilon > 0$. For this problem $\nu = 1$, whereas $u_{LP} = 2 - \epsilon$. Therefore, as $\epsilon \to 0$, $u_{LP} \to 2\nu$.

4.3 Outer Polyhedral Approximations

In this section, our results will be established based on the hierarchy of outer polyhedral approximations defined in (2.10) in Chapter 2. If $(\text{Out})_r$ defined in (3.10) is restated for the first copositive formulation of 0-1 knapsack problem, it can be given as

$$
\begin{aligned}
(\text{Out})_r^1 \quad u_r^1 := \quad \max \quad & c^T x \\
\text{s.t.} \quad & a^T x + \theta = b, && (4.4)\\
& a^T X a + 2a^T v + \omega = b^2, && (4.5)\\
& x_i + s_i = 1, \quad i = 1, \ldots, n && (4.6)\\
& X_{ii} + 2R_{ii} + S_{ii} = 1, \quad i = 1, \ldots, n, && (4.7)\\
& X_{ii} = x_i, \quad i = 1, \ldots, n && (4.8)\\
& M = \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix}, && (4.9)\\
& M \in \mathcal{O}_r, && (4.10)
\end{aligned}
$$

where $r \in \mathbb{N}$. Similarly, outer polyhedral approximations arising from $(\text{KP-CP})^2$ is given by

$$
\begin{aligned}
(\text{Out})_r^2 \quad u_r^2 := \quad \max \quad & c^T x \\
\text{s.t.} \quad & a^T x + \theta = b, && (4.11)\\
& a^T X a + 2a^T v + \omega = b^2, && (4.12)\\
& x_i + s_i = 1, \quad i = 1, \ldots, n && (4.13)\\
& R_{ii} = 0, \quad i = 1, \ldots, n, && (4.14)\\
& X_{ii} = x_i, \quad i = 1, \ldots, n && (4.15)\\
& S_{ii} = s_i, \quad i = 1, \ldots, n && (4.16)\\
& M = \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix}, && (4.17)\\
& M \in \mathcal{O}_r, && (4.18)
\end{aligned}
$$

where $r \in \mathbb{N}$. It is easy to verify that $(\text{Out})_r^2$ constitutes a tighter outer approximation than $(\text{Out})_r^1$, i.e.,

$$\text{Feas}(\text{Out})_r^2 \subseteq \text{Feas}(\text{Out})_r^1, \quad r \in \mathbb{N}. \tag{4.19}$$

Since (KP) is a maximization problem, for a given instance of (KP), (3.9) implies that

$$u_0^1 \geq u_1^1 \geq \ldots \geq \nu \quad \text{and} \quad u_0^2 \geq u_1^2 \geq \ldots \geq \nu.$$

Also, (4.19) implies that

$$u_r^1 \geq u_r^2, \quad \text{for all } r \in \mathbb{N}.$$

Furthermore, by Proposition 2, if the dual of $(\text{KP-CP})^1$ (resp. $(\text{KP-CP})^2$) has a strictly feasible solution and an attainable optimal solution, then

$$\lim_{r\to\infty} u_r^1 = \nu \text{ (resp. } \lim_{r\to\infty} u_r^2 = \nu).$$

F_r defined in (3.12) can also be restated for knapsack as follows:

$$F_r^i := \left\{ (x, s, \theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} : \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \text{Feas}(\text{Out})_r^i \right\},$$

where $i = 1, 2$ and $r \in \mathbb{N}$. Since the values of s and θ are determined by x, i.e., $s = e^n - x$ and $\theta = b - a^T x$, dimension of F_r^i can even be reduced more for the 0-1 knapsack problem. Therefore, we will redefine F_r^i as follows:

$$F_r^i := \left\{ x \in \mathbb{R}^n : \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \text{Feas}(\text{Out})_r \right\},$$

where $i = 1, 2$ and $r \in \mathbb{N}$. By (4.19),

$$F_r^2 \subseteq F_r^1, \quad r \in \mathbb{N} \tag{4.20}$$

holds trivially. Now, observe that the following problem is equivalent to $(\text{Out})_r^i$:

$$u_r^i = \max\{c^T x : x \in F_r^i\}, \tag{4.21}$$

where $i = 1, 2$ and $r \in \mathbb{N}$. By Lemma 4, we already know that $F_r \subseteq \text{Feas}(\text{Rel}(\text{KP}))$, which implies that $u_r^2 \leq u_r^1 \leq u_{LP}$, $r \in \mathbb{N}$.

4.3.1 Level 0

In this section, our aim is to compare the feasible regions F_0^1, F_0^2 and Feas(Rel(KP)). Next proposition establishes the equality of these three sets by using Theorem 3.

Proposition 8. *Given an instance of* (KP), $F_0^1 = F_0^2 = \text{Feas}(\text{Rel}(\text{KP}))$. *As a result,* $u_0^1 = u_0^2 = u_{LP}$.

Proof. We will show that $F_0^2 = \text{Feas}(\text{Rel}(\text{KP}))$ and then all assertions follow trivially. Let us put (KP) in the form of (MBP), or equivalently, consider $(\text{KP})_{aug}$ with slacks s_i, $i = 1, \ldots, n$ treated as binary. Let also A, T, I^+ and I^- be defined as in (3.20), (3.21) and (3.22), respectively. Observe that $I^- = \emptyset$ and T can always be put into the form (3.23) for all (KP) instances. Therefore, by Theorem 3, we conclude that $F_0^2 = \text{Feas}(\text{Rel}(\text{KP}))$, which implies that $F_0^1 = F_0^2 = \text{Feas}(\text{Rel}(\text{KP}))$ together with (4.20) and Lemma 4. $u_0^1 = u_0^2 = u_{LP}$ follows trivially from (4.21). □

Proposition 8 shows that at level $r = 0$, upper bounds given by the outer polyhedral approximations of $(\text{KP-CP})^1$ and $(\text{KP-CP})^2$ are exactly equal to upper bound given by the LP relaxation of (KP). We will embody the proof of Proposition 8 with the following example.

Example 13. *Consider an instance of* (KP). *Let*

$$a = \begin{bmatrix} 3 & 2 \end{bmatrix}.$$

For brevity, we will not write the other problem parameters, since they are not necessary to justify our claim. If we put (KP) *of the form* (MBP) *(or, equivalently, consider* $(\text{KP})_{aug}$*) and A is defined as in* (3.20), *then*

$$A = \begin{bmatrix} 3 & 2 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix}.$$

Accordingly, T defined in (3.21) *is*

$$T = \begin{bmatrix} 6 & 0 & 0 & 3 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

By changing the order of the columns of T, observe that it can be put in the form (3.23) *as follows:*

$$\begin{bmatrix} 6 & 0 & 0 & 3 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

where

$$D_1 = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad G = \begin{bmatrix} 3 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Observe that D_2 does not exist, since $I^- = \emptyset$. Also, observe that the argument in Proposition 8 *can be extended to all instances of* (KP) *in a similar manner.*

4.3.2 Higher Levels

In this section, we will establish that the equality between F_r^i, $i = 1, 2$ and Feas(Rel(KP)) exists not only at level 0, but until at least a certain level of $r \in \mathbb{N}$.

It is already known by Lemma 4 that $F_r^i \subseteq$ Feas(Rel(KP)) for all $i = 1, 2$ and $r \in \mathbb{N}$. Note that Feas(Rel(KP)) is a bounded polyhedron due to the constraints $0 \leq x_i \leq 1$, $i = 1, \ldots, n$, and each F_r^i, $i = 1, 2$, $r \in \mathbb{N}$, is a convex set. Therefore, by Corollary 1, a sufficient and necessary condition for the equality between F_r^2 and Feas(Rel(KP)) is to show that for an arbitrary $\hat{x} \in \mathcal{E}$(Feas(Rel(KP))), $\hat{x} \in F_r^2$ holds for a certain $r \in \mathbb{N}$. After showing $F_r^2 =$ Feas(Rel(KP)) for a certain $r \in \mathbb{N}$, $F_r^1 =$ Feas(Rel(KP)) follows trivially from Lemma 4 and (4.20).

We will use a constructive proof method to show the related assertion. If $\hat{x} \in$ Conv(Feas(KP)) (or, equivalently $\hat{x}$ has no fractional value), then the assertion follows trivially by Lemma 4. Otherwise, observe that $\hat{x}$ will have exactly one fractional value by Lemma 7. For this case, we will construct a matrix $M \in \text{Feas(Out)}_r^2$, x-component of which is equal to $\hat{x}$ at a certain level $r \in \mathbb{N}$. However, this is not an easy task since, as r increases, $\mathcal{O}_r$ will have many extreme rays with different structures. Hopefully, we can pick a subset of these rays and by using them, we show that we can construct such a matrix.

In the following section, we attempt to give the reader an insight into our construction technique.

A Discussion on Our Construction Method

In this section, we provide the technical details about the construction technique we devised. This construction technique will heavily exploit the special structure of the extreme points of the feasible region of Rel(KP). A nice aspect of our technique is that it works for $(\text{Out})_r^2$ and therefore for $(\text{Out})_r^1$ as well.

Let

$$\mathcal{E}^- = \mathcal{E}(\text{Feas}(\text{Rel}(\text{KP}))) \setminus \text{Conv}(\text{Feas}(\text{KP})). \tag{4.22}$$

Given $\hat{x} \in \mathcal{E}^-$, let us recall that our aim is to construct a matrix $M \in \text{Feas}(\text{Out})_r^2$, x-component of which is equal to $\hat{x}$ at a certain level $r \in \mathbb{N}$. While constructing such an M, elements of the X-component must be picked carefully. Inspired by $\hat{x}\hat{x}^T$, we will propose a special structure for the X-component. Since $\hat{x}$ has exactly one fractional element,

$$\begin{bmatrix} 1 \\ \hat{x} \end{bmatrix} \begin{bmatrix} 1 \\ \hat{x} \end{bmatrix}^T = \begin{bmatrix} 1 & e^k & \hat{x}_{k+1} & 0^{1\times(n-k-1)} \\ (e^k)^T & e^k(e^k)^T & \hat{x}_{k+1}e^k & 0^{k\times(n-k-1)} \\ \hat{x}_{k+1} & \hat{x}_{k+1}(e^k)^T & (\hat{x}_{k+1})^2 & 0^{1\times(n-k-1)} \\ 0^{(n-k-1)\times 1} & 0^{(n-k-1)\times k} & 0^{(n-k-1)} & 0^{(n-k-1)\times(n-k-1)} \end{bmatrix}, \tag{4.23}$$

where $e^k \in \mathbb{R}^k$ and $\hat{x}_{k+1}$ corresponds to the fractional element of $\hat{x}$. A property of $\hat{x}\hat{x}^T$ is that $a^T\left(\hat{x}\hat{x}^T\right)a = b^2$.

Now, due to constraint (4.5), we want X-component of M to satisfy $a^TXa \leq b^2$, because, this way we can always satisfy (4.5) by freely increasing the ω-component of M without violating other constraints. Therefore, while $a^T\left(\hat{x}\hat{x}^T\right)a = b^2$, $a^TXa \leq b^2$ must be satisfied. However, considering the X-component of M, due to constraint (4.8), $X_{k+1,k+1} = \hat{x}_{k+1}$ must also be satisfied. Note that $(k+1)^{th}$ diagonal of X is $\hat{x}_{k+1}$, whereas that of $\hat{x}\hat{x}^T$ is $(\hat{x}_{k+1})^2$. This gives X, from the start, a disadvantage equal to the amount $a_{k+1}^2\hat{x}_{k+1}(1-\hat{x}_{k+1}) > 0$. To compensate this, some parts of X should be entrywise less than $\hat{x}\hat{x}^T$, since $a \in \mathbb{R}_+^n$. At this very point, by focusing on the $(k+1)^{th}$ column of $\hat{x}\hat{x}^T$, we achieved to find a threshold matrix that, if not exceeded by X, ensures that $a^TXa \leq b$.

Let us define the following:

$$\bar{X} := \begin{bmatrix} e^k(e^k)^T & (1/2)\hat{x}_{k+1}e^k & 0^{k\times(n-k-1)} \\ (1/2)\hat{x}_{k+1}(e^k)^T & x_{k+1} & 0^{1\times(n-k-1)} \\ 0^{(n-k-1)\times k} & 0^{(n-k-1)} & 0^{(n-k-1)\times(n-k-1)} \end{bmatrix} \in \mathcal{S}^n, \tag{4.24}$$

Now, we will give the following lemma that will be very helpful for us in establishing the main results of this chapter regarding the outer polyhedral approximations.

Lemma 9. *Consider an instance of* (KP). *Given* $\hat{x} \in \mathcal{E}^-$, *let* $\bar{X} \in \mathbb{R}^n$ *be defined as in* (4.24). *Then,* $a^T \bar{X} a \leq b^2$ *holds.*

Proof. Since $a^T \hat{x} = b$, $a^T \left(\hat{x}\hat{x}^T\right) a = b^2$. Therefore, it suffices to show that

$$a^T \left(\hat{x}\hat{x}^T\right) a - a^T \bar{X} a = a^T \left(\hat{x}\hat{x}^T - \bar{X}\right) a = \hat{x}_{k+1} a_{k+1} \left(\sum_{i=1}^{k} a_i\right) + a_{k+1}^2 (\hat{x}_{k+1}^2 - \hat{x}_{k+1}) \geq 0.$$

First, we will evaluate the first term:

$$\begin{aligned} \hat{x}_{k+1} a_{k+1} \left(\sum_{i=1}^{k} a_i\right) &= \underbrace{\left(\frac{b - \sum_{i=1}^{k} a_i}{a_{k+1}}\right)}_{=\hat{x}_{k+1}} a_{k+1} \left(\sum_{i=1}^{k} a_i\right), \\ &= \left(b - \sum_{i=1}^{k} a_i\right) \left(\sum_{i=1}^{k} a_i\right), \end{aligned}$$

and the second term is equal to

$$\begin{aligned} a_{k+1}^2 (\hat{x}_{k+1}^2 - \hat{x}_{k+1}) &= {a_{k+1}}^2 \underbrace{\left(\frac{b - \sum_{i=1}^{k} a_i}{a_{k+1}}\right)}_{=\hat{x}_{k+1}} \underbrace{\left(\frac{b - \sum_{i=1}^{k} a_i - a_{k+1}}{a_{k+1}}\right)}_{=\hat{x}_{k+1}-1}, \\ &= \left(b - \sum_{i=1}^{k} a_i\right) \left(b - \sum_{i=1}^{k} a_i - a_{k+1}\right). \end{aligned}$$

Therefore,

$$\hat{x}_{k+1} a_{k+1} \left(\sum_{i=1}^{k} a_i\right) + a_{k+1}^2 (\hat{x}_{k+1}^2 - \hat{x}_{k+1}) = \underbrace{\left(b - \sum_{i=1}^{k} a_i\right)}_{\geq 0} \underbrace{(b - a_{k+1})}_{\geq 0} \geq 0.$$

Hence, we conclude that $a^T \bar{X} a \leq b^2$. □

According to this lemma, as long as the X-component of M is entrywise less than or equal to $\bar{X}$, we know that $a^T X a \leq b$ is always satisfied.

Having established such a threshold matrix, we also want to discuss which vectors seem reasonable to be used in the construction of $M \in \text{Feas(Out)}_r^2$, x-component of which is equal to $\hat{x}$ at a certain level $r \in \mathbb{N}$. Let us illustrate this with an example for a better understanding. Suppose $n = 4$. Consider the vectors that belong to $\Theta(n+1, 19)$, where $\Theta(n, r)$ is defined as in (2.8). Let $f(z) := zz^T - \text{Diag}(z)$, where $z \in \mathbb{N}^n$. For instance, consider the vector

$$(z^1)^T = \begin{bmatrix} 1 & 5 & 5 & 5 & 5 \end{bmatrix} \in \Theta(n+1, 19).$$

The extreme ray of $\mathcal{O}_{19}$ defined by z^1 is given by

$$\text{ext}(z^1) := \lambda f(z^1) = \lambda \begin{bmatrix} 0 & 5 & 5 & 5 & 5 \\ 5 & 20 & 25 & 25 & 25 \\ 5 & 25 & 20 & 25 & 25 \\ 5 & 25 & 25 & 20 & 25 \\ 5 & 25 & 25 & 25 & 20 \end{bmatrix}, \quad \lambda \geq 0.$$

Consider $\text{ext}(z^1)_{1,2:5}$ as the x-component and $\text{ext}(z^1)_{2:5,2:5}$ as the X-component of M. Note that using such extreme rays will disrupt the balance against the constraint $X_i = x_{ii}$, $i = 1, \ldots, n$, as $\text{ext}(z^1)$ overcharges X_{ii} compared to x_i and bulks out all entries of X relatively.

Next, consider the vector

$$(z^2)^T = \begin{bmatrix} 9 & 3 & 3 & 3 & 3 \end{bmatrix} \in \Theta(n+1, 19).$$

The extreme ray of $\mathcal{O}_{19}$ defined by z^2 is given by

$$\text{ext}(z^2) := \lambda f(z^2) = \lambda \begin{bmatrix} 72 & 27 & 27 & 27 & 27 \\ 27 & 6 & 9 & 9 & 9 \\ 27 & 9 & 6 & 9 & 9 \\ 27 & 9 & 9 & 6 & 9 \\ 27 & 9 & 9 & 9 & 6 \end{bmatrix}, \quad \lambda \geq 0.$$

Using such extreme rays overcharges the first row and first column, and disrupts the balance against the constraint $M_{11} = 1$; although they seem to work in favor of the constraint (4.5) by keeping the entries of X-component relatively small.

Observe that, except the first element, all other entries of z^1 and z^2 are equal. Fluctuating them also does not seem reasonable, as x-component of $M \in \text{Feas(Out)}_r^2$ will be mostly composed of ones (see, e.g. first row of (4.23)).

Finally, we consider the following vector:

$$(z^3)^T = \begin{bmatrix} 5 & 4 & 4 & 4 & 4 \end{bmatrix} \in \Theta(n+1, 19).$$

The extreme ray of $\mathcal{O}_{19}$ defined by z^3 is given by

$$\text{ext}(z^3) := \lambda f(z^3) = \lambda \begin{bmatrix} 20 & 20 & 20 & 20 & 20 \\ 20 & 12 & 16 & 16 & 16 \\ 20 & 16 & 12 & 16 & 16 \\ 20 & 16 & 16 & 12 & 16 \\ 20 & 16 & 16 & 16 & 12 \end{bmatrix}, \quad \lambda \geq 0.$$

$\text{ext}(z^3)$ constitutes a quite good balance between the constraints $M_{11} = 1$ and (4.5); while still keeping the X-component relatively small and thus working in favor of the constraint (4.8).

After such an observation, we state that our construction method will employ the vectors of the following form in general:

$$z^T = \left[\ (p+1) \ \middle| \ p(e^{k+1})^T \ (0^{n-k-1})^T \ \middle| \ (0^{k+1})^T \ p(e^{n-k-1})^T \ \middle| \ 0 \ \right] \in \Theta(2n+2, p(n+1)-1)$$

for some $p \in \mathbb{N}$. For such vectors, we will always ensure that $z_i z_{i+n} = 0$, $i = 2, \ldots, n+1$, which also ensures that constraint (4.14) ($R_{ii} = 0$, $i = 1, \ldots, n$) is always satisfied.

Main Results on Outer Polyhedral Approximations

By employing our construction method discussed in the previous section, we present one of the most important results of this chapter in the following theorem.

Theorem 7. *Given an instance of* (KP), $F_r^1 = F_r^2 = \text{Feas}(\text{Rel}(\text{KP}))$ *for all* $r = 0, 1, \ldots, 3n+2$. *As a result* $u_r^1 = u_r^2 = u_{LP}$, *for all* $r = 0, 1, \ldots, 3n+2$.

Proof. Let us pick an arbitrary $\hat{x} \in \mathcal{E}(\text{Feas}(\text{Rel}(\text{KP})))$. We will show that $\hat{x} \in F_r^2$ at $r = 3n+2$. To do that we will construct a matrix $M \in \text{Feas}(\text{Out})^2_{(3n+2)}$, whose x-component is equal to $\hat{x}$. If $\hat{x} \in \text{Conv}(\text{Feas}(\text{KP}))$, then $\hat{x} \in F^2_{3n+2}$ follows trivially. Therefore, suppose $\hat{x} \in \mathcal{E}^-$, where $\mathcal{E}^-$ is defined in (4.22). Then $\hat{x}$ is of the form (4.2) with exactly one fractional value.

Let $z \in \mathbb{R}^{2n+2}$ be partitioned as

$$z^T = \left[\begin{array}{c|c|c|c} v_0 & v_1^T & v_2^T & v_3 \end{array}\right], \tag{4.25}$$

where $v_0,\ v_3 \in \mathbb{R}$ and $v_1,\ v_2 \in \mathbb{R}^n$. Let $\bar{n} := 2n+2$. To construct $M \in \text{Feas}(\text{Out})^2_{(3n+2)}$, we will use the following vectors, which all belong to $\Theta(\bar{n}, 3n+2)$:

$$
\begin{aligned}
(z^1)^T &= \left[\, 4 \,\middle|\, 3(e^{k+1})^T \; (0^{n-k-1})^T \,\middle|\, (0^{k+1})^T \; 3(e^{n-k-1})^T \,\middle|\, 0 \,\right], \\
(z^2)^T &= \left[\, 4 \,\middle|\, 3(e^{k})^T \; (0^{n-k})^T \,\middle|\, (0^{k})^T \; 3(e^{n-k})^T \,\middle|\, 0 \,\right], \\
(z^3)^T &= \left[\, 4 \,\middle|\, 6(e^{k})^T \; (0^{n-k})^T \,\middle|\, (0^{k+1})^T \; 6(e^{n-k-1})^T \,\middle|\, 0 \,\right], \\
(z^4)^T &= \left[\, (n+2) \,\middle|\, (0^{k})^T \; (2n+2) \; (0^{n-k-1})^T \,\middle|\, (0^{n})^T \,\middle|\, 0 \,\right], \\
(z_i^5)^T &= \left[\, 0 \,\middle|\, (r+2)(e_i)^T \,\middle|\, (0^{n})^T \,\middle|\, 0 \,\right], \quad i = 1, \ldots, n, \\
(z_i^6)^T &= \left[\, 0 \,\middle|\, (0^{n})^T \,\middle|\, (r+2)(e_i)^T \,\middle|\, 0 \,\right], \quad i = 1, \ldots, n, \\
(z^7)^T &= \left[\, 0 \,\middle|\, (0^{n})^T \,\middle|\, (0^{n})^T \,\middle|\, r+2 \,\right],
\end{aligned}
$$

where k is defined as in (4.3) depending on $\hat{x}$, $e^k \in \mathbb{R}^k$ is the vector of all ones and $e_i \in \mathbb{R}^n$ is the i^{th} unit vector. Notice that summation of the entries of z^3 is equal to $6n-2$. Therefore, $z^3 \in \Theta(\bar{n}, 6n-4)$. However, since $6n-4 \geq 3n+2$ holds when $n \geq 2$, then $\Theta(\bar{n}, 6n-4) \subseteq \Theta(\bar{n}, 3n+2)$. This implies $z^3 \in \Theta(\bar{n}, 3n+2)$ for $n \geq 2$. Note that summation of the entries of other vectors is equal to $3n+4$, thus they are all in the set $\Theta(\bar{n}, 3n+2)$.

Let $f(z) := zz^T - \text{Diag}(z)$. Let us define

$$
\hat{M} := \frac{\hat{x}_{k+1}}{18} f(z^1) + \frac{1-\hat{x}_{k+1}}{12} f(z^2) + \frac{\hat{x}_{k+1}}{72} f(z^3) + \frac{\hat{x}_{k+1}}{6(n+1)(n+2)} f(z^4).
$$

Observe that $\hat{M}_{11} = 1$ and the (x, s)-component of $\hat{M}$ is exactly equal to $(\hat{x}, e - \hat{x})$. If we look at R-component of $\hat{M}$, $R_{ii} = 0$, $i = 1, \ldots, n$ and thus (4.14) is already satisfied. Due to constraint (4.15) and (4.16), it requires that $X_{ii} = \hat{x}_i$, $S_{ii} = 1 - \hat{x}_i$ $i = 1, \ldots, n$. Therefore, by setting $X_{ii} = \hat{x}_i$ and $S_{ii} = 1 - \hat{x}_i$, $i = 1, \ldots, n$, constraints (4.15) and (4.16) will also be satisfied. For this purpose, vectors z_i^5 and z_i^6, images of which in f affect only diagonal elements, will be used, $i = 1, \ldots, n$.

Let

$$M^* := \hat{M} + \frac{2-\hat{x}_{k+1}}{4(r+2)(r+1)}\left(\sum_{i=1}^{k} f(z_i^5) + \sum_{i=k+2}^{n} f(z_i^6)\right) + \frac{\hat{x}_{k+1}}{(n+2)(r+2)(r+1)} f(z_{k+1}^5) + \frac{1-\hat{x}_{k+1}}{2(r+2)(r+1)} f(z_{k+1}^6)$$

Note that only the diagonal elements of M^* differ from $\hat{M}$. Since M^* is constructed by the nonnegative combinations of the images of vectors $z \in \Theta(\bar{n}, 3n+2)$ in f, $M^* \in \mathcal{O}^{3n+2}$. Observe that M^* satisfies all constraints except (4.12). Observe that for X-component of M^*, $X \leq \bar{X}$ holds, where $\bar{X}$ is defined as in (4.24). Therefore, considering (X, v, ω)-component of M^*, let us define

$$\eta := a^T X a + 2a^T v + \omega = a^T X a \leq a^T \bar{X} a \leq b^2.$$

If $\eta = b^2$, then M^* satisfies all constraints and we are done. Otherwise, we will create matrix M, only different entry of which from M^* will be its last diagonal element, which will be equal to $b^2 - \eta$. M can be defined as follows:

$$M := M^* + \frac{b^2-\eta}{(r+1)(r+2)} f(z^7).$$

Observe M satisfies all the constraints of $(\text{Out})_{3n+2}$ and therefore $M \in \text{Feas}(\text{Out})^2_{3n+2}$. Since, x-component of M is exactly equal to $\hat{x}$, $\hat{x} \in F^2_{3n+2}$, which implies by Corollary 1 that $F^2_{3n+2} = \text{Feas}(\text{Rel}(\text{KP}))$. By Lemma 4 and (4.20), $F^1_r = F^2_r = \text{Feas}(\text{Rel}(\text{KP}))$ for all $r = 0, 1, \ldots, 3n+2$ and as a result, $u^1_r = u^2_r = u_{LP}$, for all $r = 0, 1, \ldots, 3n+2$. $\square$

Remark 7. *We will give an insight into the matrices constructed in the proof of* Theorem 7. *For instance, in case $k = 2$ and $n = 5$,*

$$\hat{M} = \begin{bmatrix}
1 & 1 & 1 & \hat{x}_{k+1} & 0 & 0 & 0 & 0 & (1-\hat{x}_{k+1}) & 1 & 1 & 0 \\
1 & \frac{2+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{2+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
\frac{2\hat{x}_{k+1}}{3} & \frac{\hat{x}_{k+1}}{2} & \frac{\hat{x}_{k+1}}{2} & \left(\frac{n+1}{n+2}\right)\hat{x}_{k+1} & 0 & 0 & 0 & 0 & 0 & \frac{\hat{x}_{k+1}}{2} & \frac{\hat{x}_{k+1}}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(1-\hat{x}_{k+1}) & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3-3\hat{x}_{k+1}}{4} & 0 & 0 & 0 & 0 & 0 & \frac{1-\hat{x}_{k+1}}{2} & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3-3\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{2+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{2+\hat{x}_{k+1}}{4} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

and

$$M^* = \begin{bmatrix}
1 & 1 & 1 & \hat{x}_{k+1} & 0 & 0 & 0 & 0 & (1-\hat{x}_{k+1}) & 1 & 1 & 0 \\
1 & 1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & 1 & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
\frac{2\hat{x}_{k+1}}{3} & \frac{\hat{x}_{k+1}}{2} & \frac{\hat{x}_{k+1}}{2} & \hat{x}_{k+1} & 0 & 0 & 0 & 0 & 0 & \frac{\hat{x}_{k+1}}{2} & \frac{\hat{x}_{k+1}}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(1-\hat{x}_{k+1}) & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3-3\hat{x}_{k+1}}{4} & 0 & 0 & 0 & 0 & 0 & (1-\hat{x}_{k+1}) & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3-3\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & 1 & \frac{3+\hat{x}_{k+1}}{4} & 0 \\
1 & \frac{3+\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & \frac{\hat{x}_{k+1}}{2} & 0 & 0 & 0 & 0 & \frac{3-3\hat{x}_{k+1}}{4} & \frac{3+\hat{x}_{k+1}}{4} & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

Observe that M^* satisfies all constraints except (4.12)*. However, X-component of M^* is entrywise less than or equal to $\bar{X}$ defined in* (4.24)*. Therefore, by increasing the ω-component of M^* freely,* (4.12) *can also be satisfied. This leads us to matrix M, only different entry of which from M^* is its ω-component.*

Theorem 7 clearly shows how weak outer approximations perform for the 0-1 knapsack problem. At level $r = 3n + 2$, corresponding LP problem arising from the outer approximations will have $O((2n + 2)^{3n+4})$ variables, but it still gives the same upper bound as that of the LP relaxation of (KP). Therefore, we do not recommend using outer approximations for the 0-1 knapsack problem.

Unfortunately, we cannot extend the results established for outer polyhedral approximations in Theorem 7 and the following theorems to (MBP) problem in Chapter 3. The main reason for that is that the construction procedure that we explained in the previous section exploits the special structure of the extreme points of Feas(Rel(KP)) described in Lemma 7. Recall that those extreme points can have at most one fractional points. Moreover, when one constructs a matrix $M \in \text{Feas}(\text{Out})_r^2$ (or $M \in \text{Feas}(\text{Out})_r^1$) whose x-component is equal to $\hat{x}$, observe that θ-component of M will always be equal to 0. Not having to deal with θ makes our job easier.

As for (MBP), extreme points of Feas(MBP) can have more one than fractional values and slack variables θ can also have positive and fractional values. Therefore, our construction method does not work for (MBP) and we cannot extend our results given in this chapter to this more general problem class in Chapter 3.

In the following theorem, we show that the result in Theorem 7 can be strengthened for the special case of $n = 2$.

Theorem 8. *Consider an instance of* (KP)*. Suppose* $n = 2$*.* $F_r^1 = F_r^2 = \text{Feas}(\text{Rel}(\text{KP}))$ *for all* $r = 0, 1, \ldots, 14$*. As a result* $u_r^1 = u_r^2 = u_{LP}$*, for all* $r = 0, 1, \ldots, 14$*.*

Proof. Pick an arbitrary $\hat{x} \in \mathcal{E}(\text{Feas}(\text{Rel}(\text{KP})))$. If $\hat{x} \in \text{Conv}(\text{Feas}(\text{KP}))$, then $\hat{x} \in F_{14}^2$ follows trivially. Therefore, suppose $\hat{x} \in \mathcal{E}^-$, where $\mathcal{E}^-$ is defined in (4.22). Then $\hat{x}$ is of the form (4.2). Let $z \in \mathbb{R}^{2n+2}$ be partitioned as in (4.25). Let $\bar{n} := 2n + 2 = 6$. To construct $M \in \text{Feas}(\text{Out})_r^2$ such that x-component of M is equal to $\hat{x}$, we will use the following vectors, which all belong to $\Theta(\bar{n}, 14)$:

$$
\begin{aligned}
(z^1)^T &= \left[\; 6 \; \middle| \; 5(e^{k+1})^T \; (0^{n-k-1})^T \; \middle| \; (0^{k+1})^T \; 5(e^{n-k-1})^T \; \middle| \; 0 \; \right], \\
(z^2)^T &= \left[\; 6 \; \middle| \; 5(e^{k})^T \; (0^{n-k})^T \; \middle| \; (0^{k})^T \; 5(e^{n-k})^T \; \middle| \; 0 \; \right], \\
(z^3)^T &= \left[\; 6 \; \middle| \; 10(e^{k})^T \; (0^{n-k})^T \; \middle| \; (0^{k+1})^T \; 10(e^{n-k-1})^T \; \middle| \; 0 \; \right], \\
(z^4)^T &= \left[\; 6 \; \middle| \; (0^{k})^T \; 10 \; (0^{n-k-1})^T \; \middle| \; (0^{n})^T \; \middle| \; 0 \; \right], \\
(z_i^5)^T &= \left[\; 0 \; \middle| \; (r+2)(e_i)^T \; \middle| \; (0^{n})^T \; \middle| \; 0 \; \right], \quad i = 1, \ldots, n, \\
(z_i^6)^T &= \left[\; 0 \; \middle| \; (0^{n})^T \; \middle| \; (r+2)(e_i)^T \; \middle| \; 0 \; \right], \quad i = 1, \ldots, n, \\
(z^7)^T &= \left[\; 0 \; \middle| \; (0^{n})^T \; \middle| \; (0^{n})^T \; \middle| \; r+2 \; \right],
\end{aligned}
$$

where k is defined as in (4.3) depending on $\hat{x}$, $e^k \in \mathbb{R}^k$ is the vector of all ones and $e_i \in \mathbb{R}^n$ is the i^{th} unit vector. Note that since $n = 2$ and k is defined as in (4.3), the only value k can take is equal to 1.

Similar to the proof of Theorem 7, let $f(z) := zz^T - \text{Diag}(z)$. Let

$$
\hat{M} := \frac{\hat{x}_{k+1}}{50} f(z^1) + \frac{1 - \hat{x}_{k+1}}{30} f(z^2) + \frac{\hat{x}_{k+1}}{150} \left(f(z^3) + f(z^4) \right)
$$

Note that $\hat{M}_{11} = 1$ and the (x, s)-component of $\hat{M}$ is exactly equal to $(\hat{x}, e - \hat{x})$. Due to constraints (4.15) and (4.16), it requires that $X_{ii} = \hat{x}_i \; S_{ii} = 1 - \hat{x}_i$, $i = 1, \ldots, n$.

Note that if we look at R-component of $\hat{M}$, $R_{ii} = 0$, $i = 1, \ldots, n$. Therefore, by setting $X_{ii} = \hat{x}_i$ and $S_{ii} = 1 - \hat{x}_i$, $i = 1, \ldots, n$, constraints (4.15) and (4.16) will be satisfied. For this purpose, vectors z_i^5 and z_i^6, images of which in f affect only diagonal elements, will be used, $i = 1, \ldots, n$.

Let

$$M^* = \hat{M} + \frac{1 - \hat{x}_{k+1}}{3(r+2)(r+1)} \left(\sum_{i=1}^{k} f(z_i^5) + \sum_{i=k+1}^{n} f(z_i^6) \right)$$

Note that only different elements of M^* from $\hat{M}$ are its diagonals. Since M^* is constructed by the nonnegative combinations of the images of vectors $z \in \Theta(\bar{n}, 14)$ in f, $M^* \in \mathcal{O}^{14}$. Observe that M^* satisfies all constraints except (4.12). Observe that for X-component of M^*, $X \leq \bar{X}$ holds, where $\bar{X}$ is defined as in (4.24). Therefore, considering (X, v, ω)-component of M^*, let us define

$$\eta := a^T X a + 2a^T v + \omega = a^T X a \leq a^T \bar{X} a \leq b^2.$$

If $\eta = b^2$, then M^* already satisfies all constraints and we are done. Otherwise, we will create matrix M, only different entry of which from M^* will be its last diagonal element, which will be equal to $b^2 - \eta$. M can be defined as follows:

$$M := M^* + \frac{b^2 - \eta}{(r+1)(r+2)} f(z^7).$$

Observe that M satisfies all the constraints of $(\text{Out})_{14}^2$ and therefore $M \in \text{Feas}(\text{Out})_{14}^2$. Since, x-component of M is exactly equal to $\hat{x}$, $\hat{x} \in F_{14}^2$, which implies that $F_{14}^2 = \text{Feas}(\text{Rel(KP)})$, when $n = 2$. By Lemma 4 and (4.20), $F_r^1 = F_r^2 = \text{Feas}(\text{Rel(KP)})$ for all $r = 0, 1, \ldots, 14$ and as a result, $u_r^1 = u_r^2 = u_{LP}$, for all $r = 0, 1, \ldots, 14$. □

Remark 8. *We want to give an insight into the matrices constructed in the proof of*

Theorem 8. *Since $k = 1$ and $n = 2$,*

$$\hat{M} = \begin{bmatrix} 1 & 1 & \hat{x}_{k+1} & 0 & (1-\hat{x}_{k+1}) & 0 \\ 1 & \frac{2+\hat{x}_{k+1}}{3} & \frac{\hat{x}_{k+1}}{2} & 0 & \frac{5-5\hat{x}_{k+1}}{6} & 0 \\ \hat{x}_{k+1} & \frac{\hat{x}_{k+1}}{2} & \hat{x}_{k+1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ (1-\hat{x}_{k+1}) & \frac{5-5\hat{x}_{k+1}}{6} & 0 & 0 & \frac{2-2\hat{x}_{k+1}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

and

$$M^* = \begin{bmatrix} 1 & 1 & \hat{x}_{k+1} & 0 & 1-\hat{x}_{k+1} & 0 \\ 1 & 1 & \frac{\hat{x}_{k+1}}{2} & 0 & \frac{5-5\hat{x}_{k+1}}{6} & 0 \\ \hat{x}_{k+1} & \frac{\hat{x}_{k+1}}{2} & \hat{x}_{k+1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1-\hat{x}_{k+1} & \frac{5-5\hat{x}_{k+1}}{6} & 0 & 0 & 1-\hat{x}_{k+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Observe that M^* satisfies all constraints except (4.12)*. However, X-component of M^* is entrywise less than or equal to $\bar{X}$ defined in* (4.24)*. Therefore, by increasing the ω-component of M^* freely,* (4.12) *can also be satisfied. This leads us to matrix M, only different entry of which from M^* is its ω-component.*

Note that in Theorem 7 and 8, X-component of the constructed feasible matrix was entrywise less than the threshold matrix $\bar{X}$. If we relax that restriction, we can be no more sure that (4.12) is satisfied. However, depending on the problem parameters we can achieve to get a sufficient condition, under which (4.12) is still satisfied. This sufficient condition, if satisfied, helps us improve our results even further. Note that we will still use the same classic construction technique with only one difference. This time X-component of the constructed matrix is not necessarily entrywise less than $\bar{X}$.

Given an instance of (KP), let $\hat{x} \in \mathcal{E}^-$, where $\mathcal{E}^-$ is defined in (4.22). Then, $\hat{x}$ has exactly one fractional element, and w.l.o.g., we can put it into the form (4.2). Below, depending on $\hat{x}$, we define $\tau(\hat{x})$ that lies in the center of our sufficient condition:

$$\tau(\hat{x}) := \frac{2\left(\left(\sum_{i=1}^{k} a_i\right)\left(b - \sum_{i=1}^{k} a_i\right) + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j\right)}{\left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right)} - 1, \tag{4.26}$$

where k is defined as in (4.3) depending on $\hat{x}$ of the form (4.2). First, we give the following lemma regarding $\tau(\hat{x})$.

Lemma 10. *Given an instance of* (KP)*, let* $\hat{x} \in \mathcal{E}^-$*. Let* $\tau(\hat{x})$ *be defined as in* (4.26)*. Then,* $\tau(\hat{x}) \geq 1$*.*

Proof. $\tau(\hat{x})$ in (4.26) can be rewritten as

$$\frac{2\left(\sum_{i=1}^{k} a_i\right)\underbrace{\left(b - \sum_{i=1}^{k} a_i\right)}_{>0}}{\left(b - \sum_{i=1}^{k} a_i\right)\underbrace{\left(\sum_{i=1}^{k} a_i + \underbrace{a_{k+1} - b}_{\leq 0}\right)}_{>0}} + \frac{2\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j}{\left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right)} - 1$$

Observe that first term of the summation is greater than or equal to 2, and second term is nonnegative. Therefore, we conclude that $\tau(\hat{x}) \geq 1$. $\square$

For an instance of (KP), let Ω be the set of all optimal solutions of Rel(KP). Suppose x is of the form (4.2) for all $x \in \Omega$ as Rel(KP) and all outer approximations would be exact otherwise. Since all optimal solutions are of the form (4.2) with exactly one fractional value, observe that $\Omega \subseteq \mathcal{E}^-$, where $\mathcal{E}^-$ is defined in (4.22). Let

$$\phi_{min} := (n+1)\min\{\lfloor \tau(x) \rfloor : x \in \mathcal{E}^-\} - 1 \tag{4.27}$$

and

$$\phi_{max} := (n+1)\max\{\lfloor\tau(x)\rfloor : x \in \Omega\} - 1, \tag{4.28}$$

where $\tau(x)$ is defined as in (4.26). Observe that $\phi_{min} \leq \phi_{max}$, since $\Omega \subseteq \mathcal{E}^-$.

In the next theorem, we show that depending on the problem parameters $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$, the results in Theorems 7 and 8 can even be extended further for specific instances of (KP). Combining the results in Theorems 7 and 8, following will be the last theorem of this section.

Theorem 9. *Given an instance of* (KP)*, let* Ω *be the set of all optimal solutions of* Rel(KP)*. Suppose* x *has one fractional value for all* $x \in \Omega$*. Let* ϕ_{min} *and* ϕ_{max} *be defined as in* (4.27) *and* (4.28)*, respectively. Let*

$$\nabla_1 := \begin{cases} \max\{\phi_{min}, 14\}, & \text{if } n = 2 \\ \max\{\phi_{min}, 3n+2\}, & \text{otherwise} \end{cases}$$

and

$$\nabla_2 := \begin{cases} \max\{\phi_{max}, 14\}, & \text{if } n = 2 \\ \max\{\phi_{max}, 3n+2\}, & \text{otherwise} \end{cases}$$

Then, $F_r^1 = F_r^2 = \text{Feas(Rel(KP))}$ *for all* $r = 0, 1, \ldots, \nabla_1$*. Furthermore,* $u_r^1 = u_r^2 = u_{LP}$*, for all* $r = 0, 1, \ldots, \nabla_2$*.*

Proof. Let us pick an arbitrary $\hat{x} \in \mathcal{E}^-$, where $\mathcal{E}^-$ is defined in (4.22). Then, $\hat{x}$ is of the form (4.2) with one fractional value. Let $p := \lfloor\tau(\hat{x})\rfloor$, where $\tau(\hat{x})$ is defined in (4.26). Let $\bar{r} := (n+1)p - 1$. We will show that $\hat{x} \in F_{\bar{r}}^2$. To achieve that, we will construct a matrix $M \in \text{Feas(Out)}_{\bar{r}}^2$, whose x-component is equal to $\hat{x}$. Let $z \in \mathbb{R}^{2n+2}$ be partitioned as in (4.25). Let $\bar{n} := 2n+2$. To construct $M \in \text{Feas(Out)}_{\bar{r}}^2$, we will use the following vectors, which all belong to $\Theta(\bar{n},\bar{r})$:

$$(z^1)^T = \left[\ (p+1)\ \middle|\ p(e^{k+1})^T\ (0^{n-k-1})^T\ \middle|\ (0^{k+1})^T\ p(e^{n-k-1})^T\ \middle|\ 0\ \right],$$
$$(z^2)^T = \left[\ (p+1)\ \middle|\ p(e^{k})^T\ (0^{n-k})^T\ \middle|\ (0^{k})^T\ p(e^{n-k})^T\ \middle|\ 0\ \right],$$
$$(z_i^3)^T = \left[\ 0\ \middle|\ (r+2)(e_i)^T\ \middle|\ (0^n)^T\ \middle|\ 0\ \right], \quad i=1,\dots,n,$$
$$(z_i^4)^T = \left[\ 0\ \middle|\ (0^n)^T\ \middle|\ (r+2)(e_i)^T\ \middle|\ 0\ \right], \quad i=1,\dots,n,$$
$$(z^5)^T = \left[\ 0\ \middle|\ (0^n)^T\ \middle|\ (0^n)^T\ \middle|\ r+2\ \right],$$

where k is defined as in (4.3) depending on $\hat{x}$, $e^k \in \mathbb{R}^k$ is the vector of all ones and $e_i \in \mathbb{R}^n$ is the i^{th} unit vector.

Let $f(z) := zz^T - \mathrm{Diag}(z)$. Let

$$\hat{M} := \frac{\hat{x}_{k+1}}{p^2+p} f(z^1) + \frac{1-\hat{x}_{k+1}}{p^2+p} f(z^2)$$

Note that $\hat{M}_{11} = 1$ and the (x,s)-component of $\hat{M}$ is exactly equal to $(\hat{x}, e-\hat{x})$. Due to constraints (4.15) and (4.16), $X_{ii} = \hat{x}_i$, $S_{ii} = 1-\hat{x}_i$, $i=1,\dots,n$ should be satisfied. Note that if we look at the R-component of $\hat{M}$, $R_{ii} = 0$, $i=1,\dots,n$. Hence, by setting $X_{ii} = \hat{x}_i$ and $S_{ii} = 1-\hat{x}_i$, $i=1,\dots,n$, constraints (4.15) and (4.16) will be satisfied. To achieve that, vectors z_i^3 and z_i^4, images of which in f affect only diagonal elements, will be used, $i=1,\dots,n$.

Let

$$M^* := \hat{M} + \frac{2}{(p+1)(r+2)(r+1)} \left(\sum_{i=1}^n \hat{x}_i f(z_i^3) + \sum_{i=1}^n (1-\hat{x}_i) f(z_i^4) \right),$$

Only different elements of M^* from $\hat{M}$ are its diagonals. Since M^* is constructed by the nonnegative combinations of the images of vectors $z \in \Theta(\bar{n},\bar{r})$ in f, $M^* \in \mathcal{O}^{\bar{r}}$. Observe that M^* satisfies all constraints except (4.5). Considering (X,v,ω)-component of M^*, let us define

$$\eta := a^T X a + 2a^T v + \omega = a^T X a.$$

Observe that if $\eta \leq b^2$, then we can increase ω-component of M^* as much as we want while still satisfying all other constraints. Therefore, if $\eta \leq b^2$ holds, then (4.5) can be satisfied by setting ω-component of M^* equal to $b^2 - \eta$. By the following equivalent inequalities, we show that $\eta \leq b^2$ indeed holds:

$$\frac{2\left(\left(\sum_{i=1}^{k} a_i\right)\left(b - \sum_{i=1}^{k} a_i\right) + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j\right)}{\left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right)} - 1 = \tau(\hat{x}) \geq \lfloor \tau(\hat{x}) \rfloor = p,$$

$$\frac{2}{p+1}\left(\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j + a_{k+1}\hat{x}_{k+1}\left(\sum_{i=1}^{k} a_i\right)\right) \geq \left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right),$$

$$\frac{2}{p+1}\left(\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j + a_{k+1}\hat{x}_{k+1}\left(\sum_{i=1}^{k} a_i\right)\right) - \left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right) \geq 0,$$

$$\frac{2}{p+1}\left(\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j + a_{k+1}\hat{x}_{k+1}\left(\sum_{i=1}^{k} a_i\right)\right) - {a_{k+1}}^2\left(\frac{b - \sum_{i=1}^{k} a_i}{a_{k+1}}\right)\left(1 - \frac{b - \sum_{i=1}^{k} a_i}{a_{k+1}}\right) \geq 0,$$

$$\frac{2}{p+1}\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j + \frac{2}{p+1}a_{k+1}\hat{x}_{k+1}\left(\sum_{i=1}^{k} a_i\right) - (a_{k+1})^2\hat{x}_{k+1}(1 - \hat{x}_{k+1}) \geq 0,$$

$$a^T\left(\hat{x}\hat{x}^T - X\right)a \geq 0,$$

$$\underbrace{a^T\left(\hat{x}\hat{x}^T\right)a}_{=b^2} - \underbrace{a^T X a}_{=\eta} \geq 0.$$

We showed that $\eta \leq b^2$ holds. If $\eta = b^2$, then M^* already satisfies all constraints and we are done. Otherwise, we will create matrix M, only different entry of which from M^* will be its last diagonal element, which will be equal to $b^2 - \eta$. M can be defined as follows:

$$M := M^* + \frac{b^2 - \eta}{(r+1)(r+2)} f(z^5).$$

Observe that M satisfies all the constraints of $(\text{Out})^2_{\bar{r}}$ and therefore $M \in \text{Feas}(\text{Out})^2_{\bar{r}}$. Since x-component of M is exactly equal to $\hat{x}$, $\hat{x} \in F^2_{\bar{r}}$. Assertions in Theorem 9 follow from the definition of ϕ_{min} and ϕ_{max}, and by combining the results in Theorem 7 and Theorem 8.

□

Remark 9. *We will give an insight into the matrices constructed in the proof of* Theorem 9. *For instance, in case $k = 2$ and $n = 5$,*

$$\hat{M} = \begin{bmatrix}
1 & 1 & 1 & \hat{x}_{k+1} & 0\;0\;0\;0 & (1-\hat{x}_{k+1}) & 1 & 1 & 0 \\
1 & \frac{p-1}{p+1} & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & \frac{p}{p+1} & 0 \\
1 & \frac{p}{p+1} & \frac{p-1}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & \frac{p}{p+1} & 0 \\
\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & \frac{p-1}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & 0 & \frac{p}{p+1}\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
(1-\hat{x}_{k+1}) & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & 0 & 0\;0\;0\;0 & \frac{(p-1)(1-\hat{x}_{k+1})}{p+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & 0 \\
1 & \frac{p}{p+1} & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p-1}{p+1} & \frac{p}{p+1} & 0 \\
1 & \frac{p}{p+1} & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & \frac{p-1}{p+1} & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

and

$$M^* = \begin{bmatrix}
1 & 1 & 1 & \hat{x}_{k+1} & 0\;0\;0\;0 & (1-\hat{x}_{k+1}) & 1 & 1 & 0 \\
1 & 1 & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & \frac{p}{p+1} & 0 \\
1 & \frac{p}{p+1} & 1 & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & \frac{p}{p+1} & 0 \\
\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & \hat{x}_{k+1} & 0\;0\;0\;0 & 0 & \frac{p}{p+1}\hat{x}_{k+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0 \\
(1-\hat{x}_{k+1}) & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & 0 & 0\;0\;0\;0 & \hat{s}_{k+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p(1-\hat{x}_{k+1})}{p+1} & 0 \\
1 & \frac{p}{p+1} & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & 1 & \frac{p}{p+1} & 0 \\
1 & \frac{p}{p+1} & \frac{p}{p+1} & \frac{p}{p+1}\hat{x}_{k+1} & 0\;0\;0\;0 & \frac{p(1-\hat{x}_{k+1})}{p+1} & \frac{p}{p+1} & 1 & 0 \\
0 & 0 & 0 & 0 & 0\;0\;0\;0 & 0 & 0 & 0 & 0
\end{bmatrix}.$$

Observe that M^* satisfies all constraints except (4.12). *Also, this time X-component of M^* is* **not** *necessarily less than or equal to $\bar{X}$ defined in* (4.24).

Considering (X, v, ω)-component of M^*, we want $a^T X a + 2a^T \underbrace{v}_{=0} + \underbrace{\omega}_{=0} = a^T X a$

to be less than or equal to b^2*. Hence,*

$$\begin{aligned}
b^2 - a^T X a &= a^T(\hat{x}\hat{x})a - a^T X a \\
&= a^T \left(\hat{x}\hat{x}^T - X\right) a \\
&= \frac{1}{p} \underbrace{\left(\frac{2\left(\left(\sum_{i=1}^{k} a_i\right)\left(b - \sum_{i=1}^{k} a_i\right) + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} a_i a_j\right)}{\left(b - \sum_{i=1}^{k} a_i\right)\left(\sum_{i=1}^{k} a_i + a_{k+1} - b\right)} - 1 \right)}_{=\tau(\hat{x})} - 1 \\
&= \frac{\tau(\hat{x})}{p} - 1.
\end{aligned}$$

This is exactly where $\tau(\hat{x})$ *comes out. In Lemma 10, we already proved* $\tau(\hat{x}) \geq 1$*. Therefore, by setting* $p = \lfloor \tau(\hat{x}) \rfloor$*,* $b^2 - a^T X a = \tau(\hat{x})/p - 1 \geq 0$ *is satisfied.*

Finally, by increasing the ω*-component of* M^* *freely,* (4.12) *can be satisfied. This leads us to matrix* M*, only different entry of which from* M^* *is its* ω*-component.*

We already know $\phi_{min} \leq \phi_{max}$ holds. For $n = 2$, there are (KP) instances, for which one of the following cases holds:

(i) $\phi_{min} \leq \phi_{max} \leq 14$

(ii) $\phi_{min} \leq 14 < \phi_{max}$

(iii) $14 < \phi_{min} \leq \phi_{max}$

Clearly, given a (KP) instance, where $n = 2$, Theorem 9 does not extend the results of Theorem 8 if (i) holds. On the other hand if (ii) or (iii) holds, then it will extend the results of Theorem 8. Note that for each of these three cases, it is possible to construct a (KP) instance that satisfies them. Similarly, for $n > 2$ there are (KP) instances, for which one of the following cases holds:

(i) $\phi_{min} \leq \phi_{max} \leq 3n + 2$

(ii) $\phi_{min} \leq 3n + 2 < \phi_{max}$

(iii) $3n + 2 < \phi_{min} \leq \phi_{max}$

Given a (KP) instance, where $n > 2$, Theorem 9 does not extend the results of Theorem 7 if (i) holds. On the other hand if (ii) or (iii) holds, then it will extend the results of Theorem 7. In the following examples, for $n > 2$, we give three different instances of (KP) that satisfy each case one by one. We will not give examples for the case $n = 2$, since they are easier to construct once the instances for $n > 2$ are constructed.

Example 14. *Consider the following instance of* (KP)*:*

$$c = \begin{bmatrix} 1 & 3 & 2 \end{bmatrix},$$
$$a = \begin{bmatrix} 6 & 2 & 1 \end{bmatrix} \quad \textit{and} \quad b = 7.$$

Accordingly, $\mathcal{E}^- = \{(1, 1/2, 0), (2/3, 1, 1)\}$*, where* $\mathcal{E}^-$ *defined as in* (4.22) *and* $\Omega = \{(2/3, 1, 1)\}$*. If we calculate* ϕ_{min} *and* ϕ_{max}*, both will be equal to 7. Therefore (i) holds, since*

$$\phi_{min} = \phi_{max} = 7 \leq 3n + 2 = 11.$$

Theorem 7 *states that* $F_r^1 = F_r^2 = \text{Feas(Rel(KP))}$ *and* $u_r^1 = u_r^2 = u_{LP}$ *for* $r = 1, \ldots, 11$*. In this case,* Theorem 9 *does not extend these results.*

Example 15. *Consider the following instance of* (KP)*:*

$$c = \begin{bmatrix} 15 & 3 & 2 \end{bmatrix},$$
$$a = \begin{bmatrix} 6 & 2 & 1 \end{bmatrix} \quad \textit{and} \quad b = 7.$$

Accordingly, $\mathcal{E}^- = \{(1, 1/2, 0), (2/3, 1, 1)\}$*, where* $\mathcal{E}^-$ *defined as in* (4.22) *and* $\Omega = \{(1, 1, 1/2)\}$*. If we calculate* ϕ_{min} *and* ϕ_{max}*, they will be equal to 7 and 19, respectively. Therefore (ii) holds, since*

$$\phi_{min} = 7 \leq 3n + 2 = 11 < \phi_{max} = 19.$$

Theorem 7 *states that* $F_r^1 = F_r^2 = \text{Feas}(\text{Rel}(\text{KP}))$ *and* $u_r^1 = u_r^2 = u_{LP}$ *for* $r = 1, \ldots, 11$. *In this case,* Theorem 9 *does not strengthen the result on* F_r^i, $i = 1, 2$, *but it strengthens the result on* u_r^i, $i = 1, 2$ *and states that* $u_r^1 = u_r^2 = u_{LP}$ *for* $r = 1, \ldots, 19$.

Example 16. *Consider the following instance of* (KP)*:*

$$c = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix},$$
$$a = \begin{bmatrix} 1 & 3 & 4 \end{bmatrix} \quad \textit{and} \quad b = 7.$$

Accordingly, $\mathcal{E}^- = \{(1, 1, 3/4), (1, 2/3, 1)\}$*, where* $\mathcal{E}^-$ *defined as in* (4.22) *and* $\Omega = \{(1, 1, 3/4)\}$. *If we calculate* ϕ_{min} *and* ϕ_{max}*, both will be equal to 35. Therefore (iii) holds, since*

$$3n + 2 = 11 \leq \phi_{min} = \phi_{max} = 35.$$

Theorem 7 *states that* $F_r^1 = F_r^2 = \text{Feas}(\text{Rel}(\text{KP}))$ *and* $u_r^1 = u_r^2 = u_{LP}$ *for* $r = 1, \ldots, 11$. *In this case,* Theorem 9 *strengthens the results on both* F_r^i *and* u_r^i, $i = 1, 2$ *and states that* $F_r^1 = F_r^2 \text{Feas}(\text{Rel}(\text{KP}))$ *and* $u_r^1 = u_r^2 = u_{LP}$ *for* $r = 1, \ldots, 35$.

After obtaining these results and realizing that outer polyhedral approximations perform poorly for the 0-1 knapsack problem, from a different perspective, we ask the following question: At each level r, does there exist an instance such that $\nu < u_{LP}$ and $u_r^1 = u_r^2 = u_{LP}$? In the following proposition, by exploiting the definition of $\tau(x)$ in (4.26), we show that no matter how high the level r is, at each level $r \in \mathbb{N}$, there exists an instance such that $\nu < u_{LP}$ and u_r^i, $i = 1, 2$, still remain equal to u_{LP} until at least that level r.

Proposition 9. *At each level* r^**, there exists an instance such that for that instance* $\nu < u_{LP}$ *holds and* $u_r^1 = u_r^2 = u_{LP}$ *for all* $r = 1 \ldots, r^*$.

Proof. At level r^*, consider the following:

$$b = r^* + 2 \tag{4.29}$$

$$\sum_{i=1}^{k} a_i = r^* + 1 \quad \text{and} \quad a_{k+1} = 2 \tag{4.30}$$

$$c_i > a_i,\ i = 1, \ldots, k, \quad c_{k+1} = 2 \quad \text{and} \quad c_i = 0,\ i = k+1, \ldots, n. \tag{4.31}$$

Construct a (KP) instance such that (4.29), (4.30) and (4.31) are satisfied. Observe that such an instance can always be constructed. Then,

$$\nu = \sum_{i=1}^{k} c_i < u_{LP} = 1 + \sum_{i=1}^{k} c_i.$$

Let x^* be an optimal solution of Rel(KP). Observe that $\tau(x^*) \geq 2r^* + 1$ and thus $\phi_{max} = 2nr^* \geq r^*$, where $\tau(x^*)$ and ϕ_{max} is defined as in (4.26) and (4.28), respectively. By Theorem 9, this implies $u_r^1 = u_r^2 = \ell_{LP}$ for all $r = 1, \ldots, r^*$. □

We can interpret this result as follows: No matter how much we increase the level $r \in \mathbb{N}$, there are still some (KP) instances such that upper bounds given by the outer polyhedral approximations do not improve and remains equal to u_{LP}. Therefore, this result is also important in terms of showing the weakness of outer polyhedral approximations from a different viewpoint.

In the following section we will continue with the doubly nonnegative relaxation of the 0-1 knapsack problem. Results that we established in the next section indicate that upper bounds given by the doubly nonnegative relaxation are much more promising than those given by outer polyhedral approximations.

4.4 Doubly Nonnegative Relaxations

In this section, we establish our results based on the doubly nonnegative relaxations of the both completely positive formulations of the 0-1 knapsack problem. If (DN) defined in (3.47) is restated for the first copositive formulation of the 0-1 knapsack problem, then

$$
\begin{aligned}
(\mathrm{DN})^1 \quad u_{DN}^1 := \quad \max \quad & c^T x \\
\text{s.t.} \quad & a^T x + \theta = b, \\
& a^T X a + 2a^T v + \omega = b^2, \\
& x_i + s_i = 1, \quad i = 1, \ldots, n \\
& X_{ii} + 2R_{ii} + S_{ii} = 1, \quad i = 1, \ldots, n, \\
& x_i = X_{ii}, \quad i = 1, \ldots, n \\
& M = \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix}, \\
& M \in \mathcal{DN},
\end{aligned}
$$

Similarly, doubly nonnegative relaxation of $(\text{KP-CP})^2$ is given by

$$
\begin{aligned}
(\mathrm{DN})^2 \quad u_{DN}^2 := \quad \max \quad & c^T x \\
\text{s.t.} \quad & a^T x + \theta = b, \\
& a^T X a + 2a^T v + \omega = b^2, \\
& x_i + s_i = 1, \quad i = 1, \ldots, n \\
& R_{ii} = 0, \quad i = 1, \ldots, n, \\
& X_{ii} = x_i, \quad i = 1, \ldots, n \\
& S_{ii} = s_i, \quad i = 1, \ldots, n \\
& M = \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix}, \\
& M \in \mathcal{DN},
\end{aligned}
$$

Note that $(\mathrm{DN})^2$ constitutes a tighter outer approximation than $(\mathrm{DN})^1$, i.e.,

$$\mathrm{Feas}(\mathrm{DN})^2 \subseteq \mathrm{Feas}(\mathrm{DN})^1, \quad r \in \mathbb{N}. \tag{4.32}$$

We rewrite F_{DN} given in (3.48) for the above doubly nonnegative relaxations of knapsack as follows:

$$F_{DN}^i := \left\{ (x, s, \theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} : \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \mathrm{Feas}(\mathrm{DN}) \right\}, \quad i = 1, 2,$$

which again can be reduced to

$$F_{DN}^i := \left\{ x \in \mathbb{R}^n : \begin{bmatrix} 1 & x & s & \theta \\ x & X & R & v \\ s & R^T & S & y \\ \theta & v^T & y^T & \omega \end{bmatrix} \in \mathrm{Feas}(\mathrm{DN}) \right\}, \quad i = 1, 2$$

since once $x \in \mathbb{R}^n$ is known, the values of s and θ will be determined by it. Note that the objective function of $(\mathrm{DN})^i$, $i = 1, 2$ is only dependent on x. Therefore, $(\mathrm{DN})^i$ is equivalent to the following problem:

$$u_{DN}^i = \max\{c^T x : x \in F_{DN}\}, \quad i = 1, 2. \tag{4.33}$$

It follows trivially by (4.32) that

$$F_{DN}^2 \subseteq F_{DN}^1 \quad \text{and} \quad u_{DN}^2 \leq u_{DN}^1. \tag{4.34}$$

By Lemma 2, we know that $F_{DN} \subseteq \mathrm{Feas}(\mathrm{Rel}(\mathrm{KP}))$. From this and (4.34), $u_{DN}^2 \leq u_{DN}^1 \leq u_{LP}$ follows directly. By using Corollary 2 in Chapter 3, in the next proposition we show that F_{DN}^i, $i = 1, 2$, does not contain any of the elements in $\mathcal{E}^-$.

Proposition 10. *Given an instance of* (KP), $F_{DN}^i \cap \mathcal{E}^- = \emptyset$ *for* $i = 1, 2$, *where* $\mathcal{E}^-$ *is defined as in* (4.22).

Proof. We will show that $F^1_{DN} \cap \mathcal{E}^- = \emptyset$. Then, $F^2_{DN} \cap \mathcal{E}^- = \emptyset$ will follow since $F^2_{DN} \subseteq F^1_{DN}$. Let us pick an arbitrary $\hat{x} \in \mathcal{E}^-$. Then $\hat{x}$ is of the form (4.2) with exactly one fractional value. We will show that case (i) in Corollary 2 holds for $(\mathrm{DN})^1$. Put (KP) in the form of (MBP), or equivalently, consider (KP_{aug}). Note that $B = \{1, \ldots, n\}$ and w.l.o.g. we can think of $(\hat{x}, \hat{s}, \hat{\theta})$ as $\hat{x}_1 = \ldots = \hat{x}_t = 1$, $\hat{x}_{t+1} = \ldots = \hat{x}_{n-1} = 0$, $0 < \hat{x}_n < 1$, $\hat{s} = e - \hat{x}$ and $\hat{\theta} = 0$. Since (KP_{aug}) will have $n+1$ equality constraints, let v_i, $i = 1, \ldots, n+1$ and w be defined as in (3.52) and (3.53), respectively. Observe that $w = (\hat{x}_n, \hat{s}, \hat{\theta}) \in \mathbb{R}^{n+2}$ and $v_1 = (a_n, 0^n, 1) \in \mathbb{R}^{n+2}$. We will show that v_1 satisfies case (i) in Corollary 2. First, observe that $(v_1)_1 = a_n > 0$, since $\hat{x}_n = \left(b - \sum_{i=1}^{t} a_i\right)/a_n$. Since $(v_i)_j (v_i)_l \geq 0$ for all $1 \leq j < l \leq n+2$, we only need to show that $(v_i)_j (v_i)_l = 0$ if $w_j w_l > 0$. Observe that since $\hat{\theta} = 0$ and $(v_1)_2 = \ldots = (v_1)_{n+1} = 0$, this requirement is satisfied. Therefore, by Corollary 2 $\hat{x} \notin F^1_{DN}$, which implies $F^1_{DN} \cap \mathcal{E}^- = \emptyset$. Therefore, we conclude that $F^i_{DN} \cap \mathcal{E}^- = \emptyset$ for $i = 1, 2$. □

Proposition 10 implies that if $\mathcal{E}^-$ is nonempty, the inclusion relationship between Feas(Rel(KP)) and F^i_{DN} not only holds strictly, i.e., $F^i_{DN} \subset$ Feas(Rel(KP)), but also no extreme point of Feas(Rel(KP)) that are not in Conv(Feas(KP)) is contained in F^i_{DN}, $i = 1, 2$. This leads to the following corollary.

Corollary 7. *If* Rel(KP) *has a non-integer unique optimal solution, then* $u^2_{DN} \leq u^1_{DN} < u_{LP}$.

Proof. Let x^* be the non-integer unique optimal solution of Rel(KP). Then, $x^* \in \mathcal{E}^-$, where $\mathcal{E}^-$ is defined as in (4.22). Clearly, by Proposition 10, for all $x \in F^i_{DN}$, $c^T x < c^T x^* = u_{LP}$, which implies together with (4.34) that $u^2_{DN} \leq u^1_{DN} < u_{LP}$. □

Corollary 7 clearly shows that if Rel(KP) has a unique optimal solution and it is in $\mathcal{E}^-$, then both doubly nonnegative relaxations of knapsack give a strictly tighter bound than Rel(KP). On the other hand, if $\mathcal{E}^-$ includes multiple optimal solutions of Rel(KP), say $x^1, x^2, \ldots, x^K$, where K is finite, then this may not be the case. Proposition 10 implies none of the points $x^1, \ldots, x^K$ are included in F_{DN}. However, it does not tell anything about convex hull of those solutions and F^i_{DN}, $i = 1, 2$, might still include a convex combination of them. The following example illustrates that we indeed need the uniqueness assumption in Corollary 7.

Example 17. *Consider the following instance of* (KP)*.*

$$\begin{aligned} c &= \begin{bmatrix} 12 & 4 & 6 & 6 \end{bmatrix}, \\ a &= \begin{bmatrix} 8 & 4 & 6 & 6 \end{bmatrix} \quad \textit{and} \quad b = 17, \end{aligned}$$

where $\nu = 18$ *with the optimal solution* $(x^*)^T = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix}$ *and* $u_{LP} = 21$*. Following optimal solutions of* Rel(KP) *are included by* $\mathcal{E}^-$*:*

$$\begin{aligned} (x^1)^T &= \begin{bmatrix} 1 & 1 & 5/6 & 0 \end{bmatrix}, \\ (x^2)^T &= \begin{bmatrix} 1 & 1 & 0 & 5/6 \end{bmatrix}, \\ (x^3)^T &= \begin{bmatrix} 1 & 3/4 & 1 & 0 \end{bmatrix}, \\ (x^4)^T &= \begin{bmatrix} 1 & 0 & 1 & 1/2 \end{bmatrix}, \\ (x^5)^T &= \begin{bmatrix} 1 & 0 & 1/2 & 1 \end{bmatrix}, \\ (x^6)^T &= \begin{bmatrix} 1 & 3/4 & 0 & 1 \end{bmatrix}. \end{aligned}$$

If we solve $(\mathrm{DN})^2$ *for this instance,* $u^2_{DN} = 21$ *with the optimal solution*

$$M^* \approx \begin{bmatrix} 1 & 1 & 0.6362 & 0.538 & 0.5379 & 0 & 0.3638 & 0.462 & 0.4621 & 0 \\ 1 & 1 & 0.6362 & 0.538 & 0.5379 & 0 & 0.3638 & 0.462 & 0.4621 & 0 \\ 0.6362 & 0.6362 & 0.6362 & 0.2651 & 0.2651 & 0 & 0 & 0.3711 & 0.3711 & 0 \\ 0.538 & 0.538 & 0.2651 & 0.538 & 0.0922 & 0 & 0.2728 & 0.0000 & 0.4457 & 0 \\ 0.5379 & 0.5379 & 0.2651 & 0.0922 & 0.5379 & 0 & 0.2728 & 0.4457 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.3638 & 0.3638 & 0 & 0.2728 & 0.2728 & 0 & 0.3638 & 0.0909 & 0.091 & 0 \\ 0.462 & 0.462 & 0.3711 & 0 & 0.4457 & 0 & 0.0909 & 0.462 & 0.0164 & 0 \\ 0.4621 & 0.4621 & 0.3711 & 0.4457 & 0 & 0 & 0.091 & 0.0164 & 0.4621 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Let $\mathtt{x}$ *be the x-component of* M^**, i.e.,* $\mathtt{x}^T = \begin{bmatrix} 1 & 0.6362 & 0.538 & 0.5379 \end{bmatrix}$*. Observe that although* $\nu < u_{LP}$*,* $u^2_{DN} = u_{LP}$ *still holds. By* Proposition 10*,* x^i*,* $i = 1, \dots, 6$ *are not included by* F_{DN}*. However, observe that* $\mathtt{x}$ *can be written as convex combination of* x^i*,* $i = 1, \dots, 6$*, such that* $\mathtt{x} = \sum_{i=1}^{6} \lambda_i x^i$*, where*

$$\lambda^T \approx \begin{bmatrix} 0 & 0 & 0.4621 & 0 & 0.1517 & 0.3862 \end{bmatrix}.$$

This also explains the reason why $u^2_{DN} = u_{LP}$*. Needless to say that* M^* *is also an optimal solution for* $(\mathrm{DN})^1$ *and* $u^1_{DN} = u^2_{DN} = u_{LP}$*.*

This example shows that the uniqueness assumption in Corollary 7 cannot be relaxed in general.

4.5 Conclusion

We investigated the outer polyhedral approximations defined in Chapter 2 and doubly nonnegative relaxation of the 0-1 knapsack problem. We compared the upper bounds given by these approximations to the upper bound given by the LP relaxation of the knapsack. We showed that upper bounds given by outer polyhedral approximations of the completely positive formulation of the 0-1 knapsack problem is equal to the optimal value of its LP relaxation until at least a certain level of r, that is $r = 3n+2$. At this level, LP problem arising from these outer approximations has already exponentially many variables. For that reason, we conclude that outer polyhedral approximations perform poorly for the 0-1 knapsack problem and thus we do not recommend using them as an approximation framework for the knapsack problem.

By establishing a sufficient condition, we also showed that depending on the instance, the equality between the upper bounds given by outer approximations and LP relaxation of the knapsack can persist in even at higher levels than $3n + 2$. In case of that sufficient condition, we also gave a closed formula about how much this level, which is higher than $3n + 2$, can rise. For the doubly nonnegative relaxations, we showed that they give strictly better bounds than the LP relaxation of knapsack if it has a non-integer unique optimal solution. We also gave an example illustrating that the uniqueness assumption cannot be relaxed in general.

Chapter 5

DOUBLY NONNEGATIVE RELAXATIONS OF STANDARD QUADRATIC PROGRAMS

5.1 Introduction

A standard quadratic optimization problem (StQP) involves minimizing a (nonconvex) quadratic form (i.e., a homogeneous quadratic function) over the unit simplex. It can be formulated as follows:

$$\text{(StQP)} \quad \nu(Q) = \min \left\{ x^T Q x : x \in \Delta_n \right\},$$

where $Q \in \mathcal{S}^n$ and $\mathcal{S}^n$ denotes the space of $n \times n$ real symmetric matrices. Here, Δ_n is the unit simplex in n-dimensional Euclidian space $\mathbb{R}^n$,

$$\Delta_n = \{x \in \mathbb{R}^n : e^T x = 1, \ x \geq 0\}. \tag{5.1}$$

and $e \in \mathbb{R}^n$ is the vector of all ones. We denote the set of optimal solutions of (StQP) by

$$\Omega(Q) = \{x \in \Delta_n : x^T Q x = \nu(Q)\}, \tag{5.2}$$

and for $x \in \Delta_n$, *support set* is given by,

$$\mathcal{P}(x) := \{j \in \{1, \ldots, n\} : x_j > 0\}. \tag{5.3}$$

The standart quadratic optimization problem was introduced by Bomze [7], who also described several properties of the problem. It has many application areas such as portfolio optimization [61], population genetics [49], evolutionary game theory [8] and maximum (weighted) clique problem [32, 68]. (StQP) can be polynomially solvable, when the instance matrix $Q \in \mathcal{S}^n$ is positive or negative semidefinite. However, since (StQP) contains maximum (weighted) clique problem as its special case, the problem is NP-hard, in general.

In this paper, we are interested in the *doubly nonnegative relaxation* of (StQP), which can be solvable in polynomial-time and will be referred to as (DN). We say that a matrix $Q \in \mathcal{S}^n$ is *(DN) exact* if it admits an exact (DN). Due to the NP-hardness of (StQP), characterization of (DN) exact matrices plays an important role in extending the polynomial-time solvable cases. Note that by Diananda's result [23], for all $Q \in \mathcal{S}^n$, where $n \leq 4$, exactness of (DN) is already a well-known fact. Therefore, our main purpose is to shed light on the instances of (StQP) that admit exact (DN) for $n \geq 5$.

This paper is organized as follows: in Section 5.2, we first define a set of convex cones and establish their common. We then present the copositive formulation and the doubly nonnegative (DNN) relaxation of (StQP). Next we establish local and global optimality conditions of (StQP). In section 5.3, we give a complete characterizations for the set of (StQP) instances with an exact DNN relaxation. Section 5.4 is devoted to identification of several families of instances with an exact DNN relaxation, all of which admit a polynomial time membership oracle. We investigate the relationship between the set of (DN) exact matrices and its subsets in Section 5.5. Finally, we conclude the chapter by summarizing our results in Section 5.6

5.2 Preliminaries

5.2.1 Convex Cones

We define the following cones in $\mathcal{S}^n$:

$$\begin{aligned}
\mathcal{N} &= \{M \in \mathcal{S}^n : M_{ij} \geq 0, \quad i = 1, \ldots, n;\ j = 1, \ldots, n\}, && (5.4)\\
\mathcal{PSD} &= \left\{M \in \mathcal{S}^n : u^T M u \geq 0, \quad \forall u \in \mathbb{R}^n\right\}, && (5.5)\\
\mathcal{COP} &= \left\{M \in \mathcal{S}^n : u^T M u \geq 0, \quad \forall u \in \mathbb{R}^n_+\right\}, && (5.6)\\
\mathcal{CP} &= \left\{M \in \mathcal{S}^n : M = \sum_{k=1}^{r} b^k (b^k)^T,\ \text{for some } b^k \in \mathbb{R}^n_+,\ k = 1, \ldots, r\right\}, && (5.7)\\
\mathcal{DN} &= \mathcal{PSD} \cap \mathcal{N}, && (5.8)\\
\mathcal{SPN} &= \{M \in \mathcal{S}^n : M = M_1 + M_2, \quad \text{for some } M_1 \in \mathcal{PSD},\ M_2 \in \mathcal{N}\}. && (5.9)
\end{aligned}$$

Each of these cones is closed, convex, full-dimensional, and pointed and the following set of inclusion relations is satisfied:

$$\mathcal{CP} \subseteq \mathcal{DN} \subseteq \left\{\begin{matrix} \mathcal{N} \\ \mathcal{PSD} \end{matrix}\right\} \subseteq \mathcal{SPN} \subseteq \mathcal{COP}. \tag{5.10}$$

We have $\mathcal{CP} = \mathcal{DN}$ and $\mathcal{SPN} = \mathcal{COP}$ if and only if $n \leq 4$ [23]. For $n \geq 5$, checking membership is NP-hard for both $\mathcal{CP}$ [25] and $\mathcal{COP}$ [69]. Each of the remaining four cones is tractable in the sense that they admit polynomial-time membership oracles.

Lemma 11. *Let $\mathcal{K}^n \in \{\mathcal{CP}, \mathcal{DN}, \mathcal{N}, \mathcal{PSD}, \mathcal{SPN}, \mathcal{COP}\}$. Then, the following relations are satisfied:*

(i) If $A \in \mathcal{K}^n$, then $A_{kk} \geq 0,\ k = 1, \ldots, n$.

(ii) $A \in \mathcal{K}^n$ if and only if $P^T A P \in \mathcal{K}^n$, where $P \in \mathbb{R}^{n \times n}$ is a permutation matrix.

(iii) $A \in \mathcal{K}^n$ if and only if $DAD \in \mathcal{K}^n$, where $D \in \mathcal{S}^n$ is a diagonal matrix with positive diagonal entries.

(iv) If $A \in \mathcal{K}^n$, then every principal $r \times r$ submatrix of A is in $\mathcal{K}^r$, $r = 1, \ldots, n$.

(v) If $A \in \mathcal{K}^n$ and $B \in \mathcal{K}^m$, then

$$A \oplus B = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \in \mathcal{K}^{n+m}. \tag{5.11}$$

In particular, $B = 0$ can be chosen.

5.2.2 Copositive Formulation and DNN Relaxation

For any $U \in \mathbb{R}^{m \times n}$ and $V \in \mathbb{R}^{m \times n}$, we define the inner product as the trace inner product given by

$$\langle U, V \rangle := \sum_{i=1}^{m} \sum_{j=1}^{n} U_{ij} V_{ij}.$$

(StQP) can be formulated as a copositive program [11], i.e., a linear optimization problem over an affine subset of the convex cone of completely positive matrices:

$$\text{(CP)} \quad \nu(Q) = \min\{\langle Q, X \rangle : \langle E, X \rangle = 1, \quad X \in \mathcal{CP}\},$$

where $X \in \mathcal{S}^n$ and $E = ee^T \in \mathcal{S}^n$ is the matrix of all ones.

By (5.10), we can replace the difficult conic constraint $X \in \mathcal{CP}$ by $X \in \mathcal{DN}$ and obtain a relaxation of (CP), or, equivalently, a relaxation of (StQP):

$$\text{(DN)} \quad \ell(Q) = \min\left\{\langle Q, X \rangle : \langle E, X \rangle = 1, \quad X \in \mathcal{DN}\right\},$$

(DN) is referred to as the *doubly nonnegative relaxation* of (StQP). It is well-known that (DN) satisfies the Slater's condition, which implies that strong duality is satisfied, where the dual formulation is given by

$$\text{(DN-D)} \quad \ell(Q) = \max\left\{y : yE + S = Q, \quad S \in \mathcal{SPN}\right\},$$

where $y \in \mathbb{R}$ and $S \in \mathcal{S}^n$. Furthermore, optimal solutions are attained in both (DN) and (DN-D).

For all $Q \in \mathcal{S}^n$, we have

$$\ell(Q) \leq \nu(Q), \tag{5.12}$$

since $\mathcal{CP} \subseteq \mathcal{DN}$. For $n \leq 4$, we have $\ell(Q) = \nu(Q)$ by Diananda's result. For $n \geq 5$, we are interested in the characterization of instances of (StQP) for which $\ell(Q) = \nu(Q)$.

The following lemma presents a simple shift invariance property that will be useful throughout the remainder of the paper.

Lemma 12. *For any $Q \in \mathcal{S}^n$ and any $\lambda \in \mathbb{R}$,*

$$\begin{aligned} \nu(Q + \lambda E) &= \nu(Q) + \lambda, &(5.13)\\ \ell(Q + \lambda E) &= \ell(Q) + \lambda. &(5.14) \end{aligned}$$

Furthermore, $\Omega(Q) = \Omega(Q + \lambda E)$.

Proof. The relations (5.13) and (5.14) immediately follow from the formulations (CP) and (DN) since $\langle Q + \lambda E, X\rangle = \langle Q, X\rangle + \lambda\langle E, X\rangle = \langle Q, X\rangle + \lambda$ for any $X \in \mathcal{S}^n$ such that $\langle E, X\rangle = 1$. The last assertion directly follows from the observation that

$$x^T(Q + \lambda E)x = x^T Qx + \lambda x^T Ex = x^T Qx + \lambda$$

for any $\lambda \in \mathbb{R}$ and $x \in \Delta_n$. □

5.2.3 *Local Optimality Conditions*

In this section, we review the local optimality conditions of (StQP). First, given $x \in \Delta_n$, let us define the following index sets:

$$\begin{aligned} P(x) &= \{j \in \{1, \ldots, n\} : x_j > 0\}, &(5.15)\\ Z(x) &= \{j \in \{1, \ldots, n\} : x_j = 0\}. &(5.16) \end{aligned}$$

Given an instance of (StQP), $x \in \mathbb{R}^n$ is a local minimizer if and only if there exists $s \in \mathbb{R}^n$ such that the following conditions are satisfied (see, e.g., [60, 43]):

$$
\begin{aligned}
Qx - \left(x^T Q x\right) e - s &= 0, && (5.17)\\
e^T x &= 1, && (5.18)\\
x &\in \mathbb{R}^n_+, && (5.19)\\
s &\in \mathbb{R}^n_+, && (5.20)\\
x_j s_j &= 0, \quad j = 1, \ldots, n, && (5.21)\\
d^T Q d &\geq 0, \quad \text{for all } d \in \mathbf{D}, && (5.22)
\end{aligned}
$$

where

$$\mathbf{D} = \left\{ d \in \mathbb{R}^n : e^T d = 0, \quad d^T Q x = 0, \quad d_j \geq 0, \quad \text{for each } j \in Z(x) \right\}, \tag{5.23}$$

and $Z(x)$ is given by (5.16). We remark that the Lagrange multiplier $\mu \in \mathbb{R}$ corresponding to the constraint $e^T x = 1$ is scaled and replaced by $x^T Q x$ in (5.17) by using (5.18) and (5.20).

Note that $\mathbf{D}$ consists of all feasible directions at x that are orthogonal to the gradient of the objective function at x. Furthermore,

$$\mathbf{D}_* = \left\{ d \in \mathbb{R}^n : e^T d = 0, \quad d_j = 0, \quad \text{for each } j \in Z(x) \right\} \subseteq \mathbf{D} \subseteq \mathbf{D}^* = \left\{ d \in \mathbb{R}^n : e^T d = 0 \right\}. \tag{5.24}$$

Note that (5.17) – (5.21) are the KKT conditions whereas (5.22) captures the second order optimality conditions. For an instance of (StQP), we say that $x \in \Delta_n$ is a *KKT point* if there exist $s \in \mathbb{R}^n$ such that the conditions (5.17) – (5.21) are satisfied.

5.2.4 Global Optimality Conditions

First, we note that the membership problem in $\mathcal{COP}$ can be cast in the form of (StQP) since $Q \in \mathcal{COP}$ if and only if $\nu(Q) \geq 0$. The following theorem establishes that checking the global optimality condition in (StQP) reduces to a membership problem in $\mathcal{COP}$. We include a short proof for the sake of completeness.

Theorem 10 (Bomze, 1992)**.** *Let $Q \in \mathcal{S}^n$ and let $x^* \in \Delta_n$. Then,*

$$x^* \in \Omega(Q) \quad \textit{if and only if} \quad Q - \left((x^*)^T Q x^*\right) E \in \mathcal{COP}. \tag{5.25}$$

Proof. Let $x^* \in \Omega(Q)$. Consider $Q' = Q - \left((x^*)^T Q x^*\right) E \in \mathcal{S}^n$. Then, by Lemma 12, $\nu(Q') = \nu\left(Q - \left((x^*)^T Q x^*\right) E\right) = \nu(Q) - \nu(Q) = 0$, which implies that $Q' \in \mathcal{COP}$.

Conversely, suppose that $Q - \left((x^*)^T Q x^*\right) E \in \mathcal{COP}$. Then, for any $x \in \Delta_n$, we have $x^T\left(Q - \left((x^*)^T Q x^*\right) E\right) x = x^T Q x - (x^*)^T Q x^* \geq 0$, which implies that $\nu(Q) = (x^*)^T Q x^*$, i.e., $x^* \in \Omega(Q)$. □

5.3 StQP Instances with Exact DNN Relaxations

In this section, we focus on the set of instances of (StQP) which admit an exact DNN relaxation. To that end, let us define

$$\mathcal{Q} := \{Q \in \mathcal{S}^n : \ell(Q) = \nu(Q)\}. \tag{5.26}$$

We will present several alternative characterizations of $\mathcal{Q}$. These characterizations will be subsequently used for identifying several sufficient conditions for membership in $\mathcal{Q}$.

First, given $x \in \Delta_n$, we define the following set of matrices:

$$\mathcal{S}_x = \{Q \in \mathcal{S}^n : x \in \Omega(Q)\} = \left\{Q \in \mathcal{S}^n : Q - \left(x^T Q x\right) E \in \mathcal{COP}\right\}, \tag{5.27}$$

i.e., $\mathcal{S}_x$ consists of all matrices $Q \in \mathcal{S}^n$ for which x is an optimal solution of the corresponding (StQP) instance. Note that the second equality in (5.27) immediately follows from Theorem 10.

For each $x \in \Delta_n$, it is easy to verify that $\mathcal{S}_x$ is a closed and convex cone in $\mathcal{S}^n$ and

$$\{\lambda E : \lambda \in \mathbb{R}\} \subseteq \mathcal{S}_x, \quad \text{for each } x \in \Delta_n. \tag{5.28}$$

Furthermore,

$$\bigcup_{x \in \Delta_n} \mathcal{S}_x = \mathcal{S}^n. \tag{5.29}$$

Next, we focus on the characterization of the set of matrices in $\mathcal{S}_x$ that admit an exact DNN relaxation, i.e.,

$$\mathcal{Q}_x = \mathcal{S}_x \cap \mathcal{Q} = \{Q \in \mathcal{S}^n : x \in \Omega(Q), \quad \ell(Q) = \nu(Q)\}. \tag{5.30}$$

The following lemma presents a complete characterization of $\mathcal{Q}_x$.

Lemma 13. *For any $x \in \Delta_n$,*

$$\mathcal{Q}_x = \left\{Q \in \mathcal{S}^n : Q - \left(x^T Q x\right) E \in \mathcal{SPN}\right\}. \tag{5.31}$$

Proof. We prove the relation (13) by showing that each set is a subset of the other one. Let $x \in \Delta_n$ and let $Q \in \mathcal{Q}_x$. By (5.30), $Q \in \mathcal{S}_x$ and $Q \in \mathcal{Q}$, i.e., $\ell(Q) = \nu(Q) = x^T Q x$. Then, since optimal solutions are attained in (DN-D), there exists $S^* \in \mathcal{SPN}$ such that $\nu(Q)E + S^* = Q$, which implies that $Q - \left(x^T Q x\right) E \in \mathcal{SPN}$.

Conversely, for a given $x \in \Delta_n$, if $Q - \left(x^T Q x\right) E \in \mathcal{SPN}$, then $Q \in \mathcal{S}_x$ by (5.10) and $\nu(Q) = x^T Q x$. Furthermore, let $y = x^T Q x$ and $S = Q - yE$. Then, (y, S) is a feasible solution of (DN-D), which implies that $\ell(Q) \geq x^T Q x = \nu(Q)$ since (DN-D) is a maximization problem. Combining this inequality with (5.12), we obtain $\ell(Q) = \nu(Q)$, i.e., $Q \in \mathcal{Q}$. We therefore obtain $Q \in \mathcal{Q}_x$. □

By Lemma 13, for any $x \in \Delta_n$ and $Q \in \mathcal{S}^n$, one can check if $Q \in \mathcal{Q}_x$ in polynomial-time. In contrast, checking if $Q \in \mathcal{S}_x$ is, in general, NP-hard. Furthermore, a complete characterization of the matrices in $\mathcal{S}_x \backslash \mathcal{Q}_x$ requires a full understanding of the set $\mathcal{COP} \backslash \mathcal{SPN}$. While there are some studies in lower dimensions (see, e.g., [1, 19, 38]), the problem still remains open in higher dimensions.

Similar to $\mathcal{S}_x$, it is easy to verify that $\mathcal{Q}_x$ is a closed convex cone and

$$\{\lambda E : \lambda \in \mathbb{R}\} \subseteq \mathcal{Q}_x, \quad \text{for each } x \in \Delta_n. \tag{5.32}$$

Next, for a given $x \in \Delta_n$, we aim to present an algebraic characterization of $\mathcal{Q}_x$. To that end, we identify the following subsets which will be building blocks for the set $\mathcal{Q}_x$:

$$\mathcal{P}_x = \left\{P \in \mathcal{PSD} : x^T P x = 0\right\} = \{P \in \mathcal{PSD} : Px = 0\} \tag{5.33}$$

$$\mathcal{N}_x = \left\{N \in \mathcal{N} : x^T N x = 0\right\} = \{N \in \mathcal{N} : N_{ij} = 0, \quad i \in P(x),\ j \in P(x)\}, \tag{5.34}$$

where $P(x)$ is defined as in (5.15).

For each $x \in \Delta_n$, note that $\mathcal{P}_x$ is a face of $\mathcal{PSD}$ and $\mathcal{N}_x$ is a polyhedral cone in $\mathcal{N}$. Furthermore, for any $w \in \Delta_n$, we have $w^T P w \geq 0$ for each $P \in \mathcal{P}_x$ and $w^T N w \geq 0$ for each $N \in \mathcal{N}_x$, which implies that

$$\mathcal{N}_x \subseteq \mathcal{Q}_x \subseteq \mathcal{S}_x, \quad \mathcal{P}_x \subseteq \mathcal{Q}_x \subseteq \mathcal{S}_x, \quad \text{for each } x \in \Delta_n. \tag{5.35}$$

The next proposition presents a complete algebraic characterization of $\mathcal{Q}_x$ by establishing a useful relation between $\mathcal{Q}_x$ and the sets $\mathcal{N}_x$ and $\mathcal{P}_x$.

Proposition 11. *For each $x \in \Delta_n$,*

$$\mathcal{Q}_x = \mathcal{P}_x + \mathcal{N}_x + \{\lambda E : \lambda \in \mathbb{R}\}, \tag{5.36}$$

where $\mathcal{P}_x$ and $\mathcal{N}_x$ are defined as in (5.33) *and* (5.34)*, respectively. Furthermore, for any decomposition of $Q \in \mathcal{Q}_x$ given by $Q = P + N + \lambda E$, where $P \in \mathcal{P}_x$ and $N \in \mathcal{N}_x$, we have $\lambda = x^T Q x = \ell(Q) = \nu(Q)$.*

Proof. Let $x \in \Delta_n$ and $Q \in \mathcal{Q}_x$. Then, by Lemma 13,

$$Q - \left(x^T Q x\right) E = P + N,$$

where $P \in \mathcal{PSD}$ and $N \in \mathcal{N}$. Therefore,

$$0 = x^T Q x - \left(x^T Q x\right)\left(x^T E x\right) = x^T P x + x^T N x,$$

where we used $x^T E x = 1$, which implies that $x^T P x = x^T N x = 0$ since both terms are nonnegative. Therefore, we obtain

$$Q = P + N + \left(x^T Q x\right) E,$$

where $P \in \mathcal{P}_x$ and $N \in \mathcal{N}_x$. It follows that $Q \in \mathcal{P}_x + \mathcal{N}_x + \{\lambda E : \lambda \in \mathbb{R}\}$.

Conversely, since $\mathcal{P}_x \subseteq \mathcal{Q}_x$, and $\mathcal{N}_x \subseteq \mathcal{Q}_x$ by (5.35), $\{\lambda E : \lambda \in \mathbb{R}\} \subseteq \mathcal{Q}_x$ by (5.32), and $\mathcal{Q}_x$ is a convex cone, it follows that $\mathcal{P}_x + \mathcal{N}_x + \{\lambda E : \lambda \in \mathbb{R}\} \subseteq \mathcal{Q}_x$, which establishes (5.36).

For the last assertion, let $Q \in \mathcal{Q}_x$ be decomposed as $Q = P + N + \lambda E$, where $P \in \mathcal{P}_x$ and $N \in \mathcal{N}_x$. Then, $x^T Q x = x^T P x + x^T N x + \lambda$, which implies that $x^T Q x = \lambda$. Since $Q \in \mathcal{Q}$ and $\mathcal{Q}_x \subseteq \mathcal{S}_x$, we obtain $\lambda = x^T Q x = \ell(Q) = \nu(Q)$. □

We remark that Proposition 11 gives a complete algebraic characterization of $\mathcal{Q}_x$ for each $x \in \Delta_n$. In addition, it gives a recipe to construct a matrix in $\mathcal{Q}_x$. Indeed, for given $x \in \Delta_n$, one simply needs to generate two matrices $P \in \mathcal{P}_x$, $N \in \mathcal{N}_x$, a real number λ, and define $Q = P + N + \lambda E$. By Proposition 11, this is necessary and sufficient to ensure that $Q \in \mathcal{Q}_x$ with $\nu(Q) = \ell(Q) = \lambda$.

Note that a matrix $P \in \mathcal{P}_x$ can easily be generated by picking a matrix $M \in \mathbb{R}^{n \times (n-1)}$ whose columns form a basis for $x^\perp$. Then, one can define $P = MRM^T$, where $R \in \mathcal{PSD}^{n-1}$. Alternatively, we next discuss that there is an even simpler procedure to generate such a matrix $P \in \mathcal{P}_x$ which eliminates the computation of a basis for $x^\perp$. To that end, we present a technical result first.

Lemma 14. *For any two vectors $u \in \mathbb{R}^n$ and $v \in \mathbb{R}^n$ such that $u^T v = 1$, we have*

$$\mathbf{R}(I - uv^T) = v^\perp, \tag{5.37}$$

$$(I - uv^T)(I - uv^T) = I - uv^T, \tag{5.38}$$

where $\mathbf{R}(\cdot)$ denotes the range space and $v^\perp$ denotes the orthogonal complement of v.

Proof. Let $w \in \mathbf{R}(I - uv^T)$. Then, there exists $z \in \mathbb{R}^n$ such that $w = (I - uv^T)z = z - (v^T z)u$. Therefore, $v^T w = v^T z - (v^T z)(v^T u) = 0$, which implies that $w \in v^\perp$.

Conversely, if $w \in v^\perp$, then $(I - uv^T)w = w - (v^T w)u = w$, which implies that $w \in \mathbf{R}(I - uv^T)$ and establishes (5.37).

The relation (5.38) can easily be verified. □

Using Lemma 14, we can present a simpler characterization of $\mathcal{P}_x$.

Lemma 15. *The following identity holds:*

$$\mathcal{P}_x = \left\{ P \in \mathcal{S}^n : P = \left(I - ex^T\right) R \left(I - xe^T\right) \text{ for some } R \in \mathcal{PSD}^n \right\}, \tag{5.39}$$

where $\mathcal{P}_x$ is given by (5.33).

Proof. Suppose that $P \in \mathcal{P}_x$. Then, $P \in \mathcal{PSD}$ and $x^T P x = 0$. Since $P \in \mathcal{PSD}$, there exists a matrix $L \in \mathbb{R}^{n \times n}$ such that $P = LL^T$. It follows that $L^T x = 0$, which implies that each column of L belongs to $x^\perp$. Since $e^T x = 1$, it follows from Lemma 14 that there exists a matrix $W \in \mathbb{R}^n$ such that $L = \left(I - ex^T\right) W$. Therefore, $P = LL^T = \left(I - ex^T\right) WW^T \left(I - xe^T\right) = \left(I - ex^T\right) R \left(I - xe^T\right)$, where $R = WW^T \in \mathcal{PSD}^n$.

Conversely, if $P = \left(I - ex^T\right) R \left(I - xe^T\right)$ for some $R \in \mathcal{PSD}^n$, then we clearly have $P \in \mathcal{PSD}$ and $x^T P x = 0$. □

It follows from Lemma 15 that it is necessary and sufficient to generate a matrix $R \in \mathcal{PSD}^n$ and define $P = \left(I - ex^T\right) R \left(I - xe^T\right)$ to ensure that $P \in \mathcal{P}_x$.

The following corollary is an immediate consequence of Proposition 11, (5.30), and (5.29).

Corollary 8. *The following relation is satisfied:*

$$\mathcal{Q} = \bigcup_{x \in \Delta_n} \mathcal{Q}_x, \tag{5.40}$$

where $\mathcal{Q}_x$ is given by (5.30).

We close this section by recalling that, for each $x \in \Delta_n$, the membership problem in $\mathcal{Q}_x$ is polynomial-time solvable. On the other hand, for a given $Q \in \mathcal{S}^n$, checking if $Q \in \mathcal{Q}$ is equivalent to checking if there exists $x \in \Delta_n$ such that $Q \in \mathcal{Q}_x$. Since the latter problem may not necessarily be polynomial-time solvable, we instead focus on explicitly identifying several classes of matrices that belong to $\mathcal{Q}$ in the next section.

5.4 Subsets of $\mathcal{Q}$

In this section, we identify several classes of matrices that belong to the set $\mathcal{Q}$ by relying on the characterizations presented in Section 5.3.

5.4.1 Minimum Entry on the Diagonal

In this section, we show that any matrix $Q \in \mathcal{S}^n$ whose minimum entry lies on the diagonal belongs to $\mathcal{Q}$. Let us denote the set of such matrices by $\mathcal{Q}_1$, i.e.,

$$\mathcal{Q}_1 = \left\{ Q \in \mathcal{S}^n : \min_{i=1,\ldots,n;j=1,\ldots,n} Q_{ij} = \min_{k=1,\ldots,n} Q_{kk} \right\}. \tag{5.41}$$

Proposition 12. *The following relation holds:*

$$\mathcal{Q}_1 \subseteq \mathcal{Q}, \tag{5.42}$$

where $\mathcal{Q}_1$ and $\mathcal{Q}$ are given by (5.41) *and* (5.26)*, respectively.*

Proof. Let $Q \in \mathcal{Q}_1$. Let us define $\lambda = \min_{i=1,\ldots,n;j=1,\ldots,n} Q_{ij} = \min_{k=1,\ldots,n} Q_{kk} = Q_{\ell\ell}$ and $N = Q - \lambda E$. Therefore, $Q = 0 + N + \lambda E$. Then, it easy to verify that $N \in \mathcal{N}_x$, where $x = e_\ell \in \mathbb{R}^n$. By Proposition 11, $Q \in \mathcal{Q}_x$, where $\mathcal{Q}_x$ is given by (5.30). The inclusion (5.42) follows. □

5.4.2 Positive Semidefinite Matrices on $e^\perp$

A matrix $Q \in \mathcal{S}^n$ is said to be positive semidefinite on $e^\perp$ if

$$d^T Q d \geq 0, \quad \forall d \in \mathbb{R}^n \text{ such that } e^T d = 0. \tag{5.43}$$

Let us accordingly define the following set:

$$\mathcal{Q}_2 = \left\{Q \in \mathcal{S}^n : d^T Q d \geq 0, \quad \forall d \in \mathbb{R}^n \text{ such that } e^T d = 0\right\} \tag{5.44}$$

Clearly, we have

$$\mathcal{PSD} + \{\lambda E : \lambda \in \mathbb{R}\} \subseteq \mathcal{Q}_2. \tag{5.45}$$

For any $Q \in \mathcal{Q}_2$, consider the corresponding (StQP) instance. It follows from (5.24) and (5.17)–(5.22) that any KKT point is a local minimizer. Furthermore, for any it is easy to verify that the objective function is convex over the feasible region, which implies that any KKT point is, in fact, a global minimizer.

In this section, we aim to establish that $\mathcal{Q}_2 \subseteq \mathcal{Q}$. First, we present a technical result, which would be useful to prove this inclusion.

Lemma 16. *For any $Q \in \mathcal{Q}_2$,*

$$\left(I - ex^T\right) Q \left(I - xe^T\right) \in \mathcal{PSD}, \quad \textit{for each } x \in \Delta_n. \tag{5.46}$$

Proof. The assertion follows directly from Lemma 14 since $e^T x = 1$ for each $x \in \Delta_n$. □

Proposition 13. *The following relation holds:*

$$\mathcal{Q}_2 \subseteq \mathcal{Q}, \tag{5.47}$$

where $\mathcal{Q}_2$ and $\mathcal{Q}$ are given by (5.44) *and* (5.26)*, respectively.*

Proof. Let $Q \in \mathcal{Q}_2$ and $x \in \Omega(Q)$. It suffices to show that $Q \in \mathcal{Q}_x$, where $\mathcal{Q}_x$ is given by (5.30). By Proposition 11, we need to construct a decomposition

$$Q = P + N + \left(x^T Q x\right) E,$$

where $P \in \mathcal{P}_x$, $N \in \mathcal{N}_x$ and $\mathcal{P}_x$ and $\mathcal{N}_x$ are given by (5.33) and (5.34), respectively.

Let us define

$$P = \left(I - ex^T\right) Q \left(I - xe^T\right).$$

By Lemma 16, $P \in \mathcal{PSD}$. Therefore,

$$P = Q - Qxe^T - ex^TQ + \left(x^TQx\right) E,$$

or equivalently,

$$Q - \left(x^TQx\right) E = P + \left(Qxe^T + Qxe^T - 2\left(x^TQx\right) E\right).$$

Let us accordingly define

$$N = Qxe^T + Qxe^T - 2\left(x^TQx\right) E.$$

We will show that $N \in \mathcal{N}_x$. Since $x \in \Omega(Q)$, x is a KKT point, i.e., there exist $s \in \mathbb{R}^n$ such that the conditions (5.17) – (5.21) are satisfied. By (5.17),

$$Qx - \left(x^TQx\right) e - s = 0,$$

which implies that

$$\begin{aligned} Qxe^T - \left(x^TQx\right) E - se^T &= 0, \\ ex^TQ - \left(x^TQx\right) E - es^T &= 0. \end{aligned}$$

It follows from these two equations that

$$\begin{aligned} N &= Qxe^T + ex^TQ - 2\left(x^TQx\right) E \\ &= se^T + \left(x^TQx\right) E + es^T + \left(x^TQx\right) E - 2\left(x^TQx\right) E \\ &= se^T + es^T. \end{aligned}$$

Finally, note that $N \in \mathcal{N}_x$ since $N \in \mathcal{N}$ and $x^TNx = 0$ by (5.18), (5.20), and (5.21). It follows from Proposition 11 that $Q \in \mathcal{Q}_x$. □

Note that the proof of Proposition 13 is based on an explicit construction of the decomposition of a matrix $Q \in \mathcal{Q}_2$ given by Proposition 11.

5.4.3 Motzkin-Strauss Family on Perfect Graphs

First, we briefly discuss the maximum weighted clique problem in undirected graphs. Let $G = (V, E)$ be a simple, undirected graph with $V = \{1, \ldots, n\}$ and let $w \in \mathbb{R}^n_+$ be strictly positive, where w_k denotes the weight of vertex $k,\ k = 1, \ldots, n$. A set $C \subseteq V$ is a clique if all pairs of vertices in C are connected by an edge. The weight of a clique $C \subseteq V$, denoted by $w(C)$, is given by $w(C) = \sum\limits_{j \in S} w_j$. The maximum weighted clique problem is concerned with finding a clique with the maximum weight, and this weight is denoted by $\omega(G, w)$. Note that the maximum weighted clique problem is equivalent to the maximum clique problem if all the weights are identical.

We next present a connection between the maximum weighted clique problem and (StQP). Consider the graph G defined above. Let us define the following class of matrices:

$$\mathcal{M}(G, w) = \left\{ B \in \mathcal{S}^n : \begin{array}{ll} B_{kk} = 1/w_k, & k = 1, \ldots, n, \\ B_{ij} = 0, & (i, j) \in E, \\ 2B_{ij} \geq B_{ii} + B_{jj}, & \text{otherwise} \end{array} \right\}. \tag{5.48}$$

The following theorem establishes the aforementioned connection.

Theorem 11 ([32], Theorem 5)**.** *Let $G = (V, E)$ be a simple, undirected graph with $V = \{1, \ldots, n\}$ and let $w \in \mathbb{R}^n_+$ be strictly positive, where w_k denotes the weight of vertex $k,\ k = 1, \ldots, n$. Then, for any $Q \in \mathcal{M}(G, w)$,*

$$\nu(Q) = \min\{x^T Q x : x \in \Delta_n\} = \frac{1}{\omega(G, w)}. \tag{5.49}$$

Theorem 11 is a generalization of the well-known Motzkin-Strauss Theorem that establishes the first connection between the maximum clique problem and a particular instance of (StQP).

We next discuss the weighted Lovász theta number. Let G be a graph with $V(G) = \{1, \ldots, n\}$ and let $w \in \mathbb{R}^n_+$ be strictly positive, where w_k denotes the weight of vertex k, $k = 1, \ldots, n$. Let $\overline{G}$ denote the graph complement of G. The weighted Lovász theta number is given by

$$\vartheta(G, w) = \max \left\{ \langle W, X \rangle : \langle I, X \rangle = 1, \quad X_{ij} = 0, \ (i,j) \in E, \quad X \in \mathcal{PSD} \right\}, \tag{5.50}$$

where $W \in \mathcal{S}^n$ is given by

$$W_{ij} = \sqrt{w_i w_j}, \ 1 \leq i \leq j \leq n. \tag{5.51}$$

The weighted Lovász theta number satisfies $\omega(G, w) \leq \vartheta(\overline{G}, w)$ [34, 56]. It turns out that

$$\omega(G, w) = \vartheta(\overline{G}, w) \quad \text{if } G \text{ is a perfect graph.} \tag{5.52}$$

Note that a graph is called *perfect graph* if neither G nor its complement contains an induced subgraph which is an odd cycle of length at least five. In [20], it has been proven that there exists a polynomial-time algorithm to recognize perfect graphs.

The weighted Lovász theta number can be strengthened by replacing the constraint $X \in \mathcal{PSD}$ by $X \in \mathcal{DN}$ [85]:

$$\vartheta'(G, w) = \max \left\{ \langle W, X \rangle : \langle I, X \rangle = 1, \quad X_{ij} = 0, \ (i,j) \in E, \quad X \in \mathcal{DN} \right\}, \tag{5.53}$$

The strengthened version of the weighted Lovász theta number satisfies the following relations:

$$\omega(G, w) \leq \vartheta'(\overline{G}, w) \leq \vartheta(\overline{G}, w). \tag{5.54}$$

By (5.52) and (5.54), it follows that

$$\omega(G, w) = \vartheta'(\overline{G}, w) \quad \text{if } G \text{ is a perfect graph.} \tag{5.55}$$

We next establish a useful connection between the strengthened version of the weighted Lovász theta number and the doubly nonnegative relaxation via the matrices that belong to $\mathcal{M}(G, w)$. Before that we will need the following definition and the lemma.

Definition 17. *For a given $Q \in \mathcal{S}^n$ a simple undirected graph $G(Q) = (V(Q), E(Q))$ is called as the* convexity graph *of Q if the set of vertices is given by $V(Q) = \{1, \ldots, n\}$ and the set of edges is defined as*

$$E(Q) = \{(i,j) : 2Q_{ij} < Q_{ii} + Q_{jj}, \quad 1 \leq i < j \leq n\}. \tag{5.56}$$

Following lemma establishes the existence of an optimal solution with a special structure in (DN) and this observation will be used in the proof of Theorem 12.

Lemma 17. *There exists an optimal solution X^* of* (DN) *such that*

$$X^*_{ij} = 0, \quad \text{if } (i,j) \notin G(Q).$$

Proof. Let X^* be an optimal solution of (DN). If X^* satisfies the claim, then we are done. Otherwise, suppose $X^*_{ij} > 0$ for some $(i,j) \notin G(Q)$. If we define,

$$X(\alpha) := X^* + \alpha(e_i - e_j)(e_i - e_j)^T.$$

Observe that $X(\alpha) \in \mathcal{DN}$ if $0 \leq \alpha \leq X^*_{ij}$. Set $\alpha = X^*_{ij}$. Observe that

$$\langle Q, X(\alpha)\rangle = \langle Q, X^*\rangle + \alpha \underbrace{(Q_{ii} + Q_{jj} - 2Q_{ij})}_{\leq 0} \leq \langle Q, X^*\rangle$$

which implies that $X(\alpha)$ is an optimal solution satisfying the claim. This completes the proof. □

Theorem 12. *For any $Q \in \mathcal{M}(G,w)$,*

$$\ell(Q) = \frac{1}{\vartheta'(\overline{G}, w)}. \tag{5.57}$$

Proof. First we will show that $\ell(Q) \leq \dfrac{1}{\vartheta'(\overline{G}, w)}$. Let X^{L+S} be an optimal solution of (5.53). Since $X^{L+S} \in \mathcal{PSD}$, $X^{L+S} = Y^TY$ for some $Y \in \mathbb{R}^{n \times n}$, which implies $X^{L+S}_{ij} = (y^i)^T y^j \geq 0$, $\forall i,j \in V$, where y^i is the i^{th} column vector of Y. Now, let

$$\hat{X} = \hat{Y}\hat{Y}^T,$$

where $\hat{Y} = [\alpha_1 y^1, \ldots, \alpha_n y^n]$ and

$$\alpha_i = \frac{\sqrt{w_i}}{\sqrt{\vartheta'(\overline{G}, w)}} \geq 0.$$

We will show that $\hat{X}$ is a feasible solution for (DN).

$$\begin{aligned}
\langle J, \hat{X} \rangle &= \sum_{i,j \in V(G)} \hat{X}_{ij} \\
&= \sum_{i,j \in V(G)} \alpha_i \alpha_j (y^i)^T y^j \\
&= \sum_{i \in V(G)} \alpha_i^2 (y^i)^T y^i + \sum_{\substack{i,j \in V(G) \\ i \neq j}} \alpha_i \alpha_j (y^i)^T y^j \\
&= \frac{1}{\vartheta'(\overline{G}, w)} \left(\sum_{i \in V(G)} w_i \underbrace{(y^i)^T y^i}_{= X_{ii}^{L+S}} + \sum_{\substack{i,j \in V(G) \\ i \neq j}} \sqrt{w_i} \sqrt{w_j} \underbrace{(y^i)^T y^j}_{= X_{ij}^{L+S}} \right) \\
&= \frac{1}{\vartheta'(\overline{G}, w)} \vartheta'(\overline{G}, w) = 1.
\end{aligned}$$

Also, observe that $\hat{X} \in \mathcal{DN}$. We showed that $\hat{X}$ is a feasible solution for (DN). Let us calculate

$$\begin{aligned}
\langle Q, \hat{X} \rangle &= \sum_{i,j \in V(G)} Q_{ij} \hat{X}_{ij} \\
&= \sum_{i \in V(G)} Q_{ii} \alpha_i^2 (y^i)^T y^i + \sum_{\substack{i,j \in V(G) \\ i \neq j}} Q_{ij} \alpha_i \alpha_j (y^i)^T y^j \\
&= \sum_{i \in V(G)} (1/w_i) \alpha_i^2 (y^i)^T y^i + \sum_{(i,j) \in E(G)} Q_{ij} \alpha_i \alpha_j \underbrace{(y^i)^T y^j}_{=0} + \sum_{(i,j) \notin E(G)} \underbrace{Q_{ij}}_{=0} \alpha_i \alpha_j (y^i)^T y^j \\
&= \sum_{i \in V(G)} (1/w_i) \alpha_i^2 (y^i)^T y^i \\
&= \frac{1}{\vartheta'(\overline{G}, w)} \underbrace{\sum_{i \in V(G)} \underbrace{(y^i)^T y^i}_{= X_{ii}^{L+S}}}_{=1}
\end{aligned}$$

Therefore, we conclude that $\ell(Q) \leq \langle Q, \hat{X} \rangle = \dfrac{1}{\vartheta'(\overline{G}, w)}$.

Now, we will show that $\frac{1}{\vartheta'(\overline{G}, w)} \leq \ell(Q)$. Due to Lemma 17, we know that there exists an optimal solution X^* of (DN) such that $X^*_{ij} = 0$ for all $(i, j) \notin E(G(Q))$. Since $X^* \in \mathcal{PSD}$, $X^* = F^T F$ for some $F \in \mathbb{R}^{n \times n}$, which implies $X^*_{ij} = (f^i)^T f^j \geq 0$, $\forall i, j \in V$, where f^i is the i^{th} column vector of F. Now, let

$$\tilde{X} = \tilde{F}\tilde{F}^T,$$

where $\tilde{F} = [\beta_1 f^1, \ldots, \beta_n f^n]$ and

$$\beta_i = \frac{1}{\sqrt{\ell(Q) w_i}} \geq 0.$$

We will show that $\tilde{X}$ is a feasible solution for (5.53). Note that $\tilde{X}_{ij} = \beta_i \beta_j X^*_{ij} = 0$, for all $(i, j) \in E(G)$, thus second constraint is already satisfied. Observe the following equalities:

$$\begin{aligned} \sum_{i \in V(G)} \tilde{X}_{ii} &= \sum_{i \in V(G)} \beta_i^2 X^*_{ii} \\ &= \frac{1}{\ell(Q)} \underbrace{\sum_{i \in V(G)} \frac{1}{w_i} X^*_{ii}}_{=\ell(Q)} = 1 \end{aligned}$$

Finally, observe that $\tilde{X} \in \mathcal{DN}$ and thus $\tilde{X}$ is a feasible solution for (5.53). If we calculate

$$\begin{aligned} \sum_{i,j \in V(G)} \sqrt{w_i} \tilde{X}_{ij} \sqrt{w_j} &= \sum_{i,j \in V(G)} \sqrt{w_i} \beta_i \beta_j X^* \sqrt{w_j} \\ &= \frac{1}{\ell(Q)} \underbrace{\sum_{i,j \in V(G)} X^*}_{=1} \end{aligned}$$

Hence, we have $\vartheta(G, w) \geq \sum_{i,j \in V} \sqrt{w_i} \tilde{X}_{ij} \sqrt{w_j} = \frac{1}{\ell(Q)}$. Combining this inequality with the previous one we conclude that for $Q \in \mathcal{M}(G, w)$, $\ell(Q) = \frac{1}{\vartheta(\overline{G}, w)}$. □

We are now in a position to establish the relation between the doubly nonnegative relaxations of standard quadratic programs and the maximum weighted clique problem. Consider the following set of matrices:

$$\mathcal{M} = \left\{ Q \in \mathcal{S}^n : \begin{array}{c} Q \in \mathcal{M}(G,w) \text{ for some } w > 0 \\ \text{and a perfect graph } G = (V,E) \end{array} \right\} \tag{5.58}$$

$$\mathcal{Q}_3 = \mathcal{M} + \{\lambda E : \lambda \in \mathbb{R}\} \tag{5.59}$$

Proposition 14. *The following relation holds:*

$$\mathcal{Q}_3 \subseteq \mathcal{Q}, \tag{5.60}$$

where $\mathcal{Q}_3$ and $\mathcal{Q}$ are given by (5.59) *and* (5.26)*, respectively.*

Proof. First we will show that $\mathcal{M} \subseteq \mathcal{Q}$. Let us pick an arbitrary $Q \in \mathcal{M}$. Since $Q \in \mathcal{M}(G,w)$, by Theorem 11 and 12, $\nu(Q) = 1/\omega(G,w)$ and $\ell(Q) = 1/\vartheta'(\overline{G},w)$, respectively. Since G is perfect graph, it follows from (5.55) that $\nu(Q) = \ell(Q)$, which implies that $Q \in \mathcal{Q}$. Therefore, we conclude that $\mathcal{M} \subseteq \mathcal{Q}$.

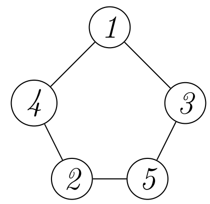
After establishing $\mathcal{M} \subseteq \mathcal{Q}$, (5.60) follows from the shift invariance property provided in Lemma 12. □

We next present an example illustrating that the perfectness assumption on G in $\mathcal{M}$ cannot be relaxed in general.

Example 18. *Let*

$$Q = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix}.$$

Observe that $Q \in \mathcal{M}(G,w)$ with the following graph G



and $w = e \in \mathbb{R}^5$. *However, G is an imperfect graph since it is an odd cycle of length five. Observe that* $\ell(Q) = 1/\sqrt{5} < \nu(Q) = 1/2$, *which implies that* $Q \notin \mathcal{Q}$.

Finally we established three different subsets of $\mathcal{Q}$. We want to stress the fact that checking membership in all the sets $\mathcal{Q}_i$, $i = 1, 2, 3$, can be done in polynomial-time.

5.5 Relations Between $\mathcal{Q}$ and Its Subsets

This section is devoted entirely to constructing examples that show the relations between $\mathcal{Q}$ and its subsets established in Section 5.4.

Our first example shows that $\mathcal{Q}_1 \setminus (\mathcal{Q}_2 \cup \mathcal{Q}_3)$ is nonempty.

Example 19. *Let*

$$Q = \begin{bmatrix} 0 & 1 & 3 & 2 & 0 \\ 1 & 3 & 1 & 3 & 2 \\ 3 & 1 & 2 & 1 & 3 \\ 2 & 3 & 1 & 1 & 0 \\ 0 & 2 & 3 & 0 & 1 \end{bmatrix}. \tag{5.61}$$

$Q \in \mathcal{Q}_1$ *since* $\min\limits_{i=1,\ldots,n; j=1,\ldots,n} Q_{ij} = Q_{11}$. *By using* Lemma 16, *it can be easily verified that* $Q \notin \mathcal{Q}_2$. *Observe that* $2Q_{12} = 2 < Q_{11} + Q_{22}$ *which implies* $Q \notin \mathcal{M}(G, w)$ *and thus* $Q \notin \mathcal{Q}_3$.

We now show that $\mathcal{Q}_2 \setminus (\mathcal{Q}_1 \cup \mathcal{Q}_3)$ is nonempty in the following example.

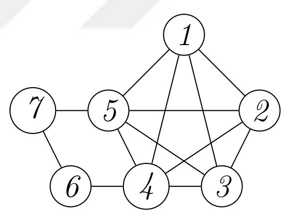
Example 20. *Let*

$$Q = \begin{bmatrix} 4 & 1 & 0 & 0 & 0 & 0 \\ 1 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 0 & 2 & 2 \end{bmatrix}.$$

Verify that $Q \in \mathcal{Q}_2$ by Lemma 16. *$Q \notin \mathcal{Q}_1$ since minimum entry of Q is not on the diagonal. $Q \notin \mathcal{Q}_3$ since $2Q_{12} = 2 < Q_{11} + Q_{22}$, which implies $Q \notin \mathcal{M}(G, w)$.*

Next example shows that $\mathcal{Q}_3 \setminus (\mathcal{Q}_2 \cup \mathcal{Q}_1)$ is nonempty.

Example 21. *Let G be given by the following graph:*



It can be verified by a polynomial-time algorithm that G is a perfect graph [20]. Let also

$$Q = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

Observe that $Q \in \mathcal{M} \subseteq \mathcal{Q}_3$ with G and $w = e \in \mathbb{R}^7$. Finally it is easily verified that $Q \notin (\mathcal{Q}_2 \cup \mathcal{Q}_1)$.

Finally, we also show in the next example that $\mathcal{Q} \setminus (\mathcal{Q}_1 \cup \mathcal{Q}_2 \cup \mathcal{Q}_3)$ is nonempty.

Example 22. *Let*

$$Q = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 4 \\ 0 & 0 & 0 & 4 & 1 \end{bmatrix}.$$

By solving (StQP) *and* (DN) *for* Q*, and checking membership in* $\mathcal{Q}_i$*,* $i = 1, 2, 3$*, it can be verified that* $Q \in \mathcal{Q} \setminus (\mathcal{Q}_1 \cup \mathcal{Q}_2 \cup \mathcal{Q}_3)$*.*

Since $\mathcal{PSD} \subseteq \mathcal{Q}_2$, both $\mathcal{Q}_2$ and $\mathcal{Q}$ have a nonempty interior. We now establish in the following proposition that $\mathcal{Q}_1$ also has a nonempty interior.

Proposition 15. $\text{int}(\mathcal{Q}_1) \subseteq \mathcal{S}^n$ *is nonempty.*

Proof. Let $Q \in \mathcal{S}^n$ such that $Q_{11} = 0$ all other elements of Q is equal to 1. Let $N \in \mathcal{S}^n$ be any matrix with $\|N\|_F := \langle N, N \rangle = 1$. Observe that $-1 \leq N_{ij} \leq 1$, for all $i = 1, \ldots, n$ and $j = 1, \ldots, n$. We will show that $Q^N = Q - \epsilon N$ is contained in $\mathcal{Q}_1$ for every N and $\epsilon \leq 1/3$. Observe that $-1/3 \leq Q^N_{11} \leq 1/3$ and $2/3 \leq Q^N_{ij} \leq 4/3$ for all $(i, j) \neq (1, 1)$. Therefore, the minimum entry of Q^N remains its first diagonal, which implies that $Q^N \in \mathcal{Q}_1$ for every N and $\epsilon \leq 1/3$. It follows that Q lies in the interior of $\mathcal{Q}_1$. Therefore, we conclude that $\mathcal{Q}_1$ has a nonempty interior. □

Showing that interior of $\mathcal{Q}_3$ is nonempty can be done by a similar argument to that in Proposition 15.

Proposition 16. $\text{int}(\mathcal{Q}_3) \subseteq \mathcal{S}^n$ *is nonempty.*

Proof. Let $Q \in \mathcal{S}^n$ such that $Q_{ii} = 1$, $i = 1 \ldots, n$, and all off-diagonal entries of Q is equal to 2. Observe that $Q \in \mathcal{M} \subseteq \mathcal{Q}_3$ with an edgeless graph G and $w = e \in \mathbb{R}^n$, since an edgeless graph is always perfect. Let $N \in \mathcal{S}^n$ be any matrix with $\|N\|_F := \langle N, N \rangle = 1$. Observe that $-1 \leq N_{ij} \leq 1$, for all $i = 1, \ldots, n$ and $j = 1, \ldots, n$. We will show that $Q^N = Q - \epsilon N$ is contained in $\mathcal{Q}_1$ for every N and $\epsilon \leq 1/3$. Observe that $2/3 \leq Q^N_{ii} \leq 4/3$ and $5/3 \leq Q^N_{ij} \leq 7/3$ for all $i = 1 \ldots, n$, $j = 1 \ldots, n$, $i \neq j$. Accordingly, $2Q^N_{ij} \geq Q^N_{ii} + Q^N_{jj}$ for all $i = 1 \ldots, n$, $j = 1 \ldots, n$, $i \neq j$. Therefore, $Q^N \in \mathcal{M} \subseteq \mathcal{Q}_3$ with the same edgeless graph G and $w_i = Q_{ii} > 0$. It follows that Q lies in the interior of $\mathcal{Q}_3$. Therefore, we conclude that $\mathcal{Q}_3$ has a nonempty interior. □

5.6 Conclusion

For a given matrix $Q \in \mathcal{S}^n$, recognizing if Q is (DN) exact is important, because one can then solve the polynomial-time solvable DNN relaxation instead of solving the NP-hard original problem and still gets the optimal value of the original problem.

In this study, we investigated the instances of (StQP) with an exact DNN relaxation. We gave a complete algebraic characterization for the set of (DN) exact matrices ($\mathcal{Q}$). By relying on the characterization of $\mathcal{Q}$, we identified three subsets of $\mathcal{Q}$, all of which are convex cones with a nonempty interior and whose membership can be checked in polynomial-time. None of the three sets is a subset of the other two sets as we showed by examples in Section 5.5. Note that there are still elements that are in $\mathcal{Q}$ and not in those subsets. Therefore, the complexity of the membership problem in $\mathcal{Q}$ is still unknown.

Chapter 6

CONCLUSION AND FUTURE RESEARCH

In this chapter, we briefly summarize our results, contributions and discuss possible directions of the future research. We also present two conjectures as our open questions.

6.1 Conclusion

In this dissertation, we investigated the quality of bounds arising from certain outer approximations of the copositive formulations of various nonconvex optimization problems. We provided Burer's copositive formulation [18] which forms the basis for this thesis. Thanks to that and the copositive formulation of Bomze et al. [11], we studied three different nonconvex optimization problems: mixed binary integer programs, 0-1 knapsack problem and standard quadratic programs. Note that in this dissertation, we do not to propose an algorithmic framework for solving copositive programs. The main aim of this thesis was to analyze the behaviour of the bounds arising from outer approximations and our theoretical results contribute in that regard.

In the introduction part, we gave a brief literature review and presented our motivation for this study. We also presented our contributions and outline of the thesis.

Chapter 2 is devoted to the copositive and completely positive optimization. We discussed the approximation hierarchies that have been proposed in the literature for the copositive and completely positive cones. The scope of this dissertation is also provided in this chapter.

In Chapter 3, we studied the outer approximations of the copositive formulations of mixed binary integer programs (MBP). We established that the lower bounds due to outer approximations are at least as good as that of LP relaxation. Although this result seems promising, we achieve to establish sufficient (or necessary) conditions indicating the weakness of outer polyhedral approximations. On the other hand, our results on doubly nonnegative (DNN) relaxations indicate that they give better lower bounds. We also discussed possible extensions of our results to the mixed binary quadratic programs.

We focused on the 0-1 knapsack problem, a special case of (MBP), in Chapter 4. We study two different copositive formulations of the 0-1 knapsack problem (KP). Since (KP) is a special case of (MBP), the results established in Chapter 3 are also valid for (KP). Additionally, it has been proven that upper bounds obtained from outer polyhedral approximations are exactly equal to the upper bound provided by the LP relaxation until at least a certain level of the hierarchy. This result clearly shows how weak outer approximations perform for the 0-1 knapsack problem. Therefore, we do not recommend using them as an approximation framework for the 0-1 knapsack problem. On the other hand, we established that if the LP relaxation of (KP) has a non-integer unique solution, then the DNN relaxations give strictly better upper bound than the LP relaxation.

Lastly, we investigated the instances of (StQP) whose DNN relaxation is exact. We gave a complete algebraic characterization for the set of (StQP) instances with an exact DNN relaxation (we call this set $\mathcal{Q}$). Furthermore, we proposed a recipe for constructing such instances of (StQP). We identified three different subsets of $\mathcal{Q}$. It turns out that the membership problem in each subset is polynomial-time solvable. We also showed that each of those three subsets have a nonempty interior. However, $\mathcal{Q}$ still has elements that are not in any of those subsets. The complexity of the membership problem in $\mathcal{Q}$ is still unknown to us at the moment of writing.

6.2 Future Work and Open Questions

Approximation hierarchies proposed for the copositive and completely positive cones do not take problem structure into account. There is an approximation algorithm proposed by Bundfuss and Dür [17] which adaptively updates itself according to the objective function of the problem. It gives very promising results for (StQP), however does not perform well for all problems under the general case of mixed binary quadratic programs.

We believe more efficient approximation approaches that also exploit the problem structure will be developed for the coposotive programs in future. We also hope this study to contribute to the refinement of the current approximations by shedding light into their strengths and weaknesses.

Finally, we would like to end this dissertation by sharing two conjectures that we have yet to prove or disprove.

Both our computational and theoretical results point to the weakness of outer polyhedral approximations and indicate that doubly nonnegative relaxations perform better. Therefore, we have the following conjecture between outer polyhedral approximations and the doubly nonnegative cone.

Conjecture 1. *$\mathcal{DN} \subseteq \mathcal{O}_r$ for all $r \leq n-2$, where $n \geq 2$.*

If Conjecture 1 is proven, its implication will set a clear distinction between the performance of outer polyhedral approximations (due to de Klerk and Pasechnik [22]) and the doubly nonnegative relaxations. It also clearly favors doubly nonnegative relaxations over outer approximations, since the resulting LP from outer approximations grows with $\mathcal{O}(n^n)$ at $r = n-2$.

Based on the results we obtained for the 0-1 knapsack problem, we have the following conjecture for (MBP) which claims that lower bounds arising from outer polyhedral approximations do not improve until at least a certain hierarchy level for

(MBP) as well. We denote these lower bounds as ℓ_r, $r \in \mathbb{N}$ and $B \subseteq \{1, \ldots, n\}$ is the index set of variables with binary restrictions. We refer the reader to Chapter 3 for the details.

Conjecture 2. *Given an* (MBP) *instance,* $\ell_0 = \ell_1 = \ldots = \ell_{|B|}$.

If Conjecture 2 is proven, it will also be a clear indication of why outer polyhedral approximations perform poorly for (MBP).

Copositive formulations enable us to treat many nonconvex, combinatorial and NP-hard optimization problems from the perspective of convex optimization. A better understanding of the intractable cones $\mathcal{CP}$, $\mathcal{COP}$, and their tractable approximations provides us with opportunities to deal with these problems more efficiently.

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