Binary Conic Quadratic Knapsacks

by

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Abstract

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Binary Conic Quadratic Knapsack set is the lower level set of the conic quadratic set functions. They are natural generalizations of linear knapsack sets, and have several applications in several areas, such as, combinatorial optimization, finance, and optimal control. In particular, conic quadratic knapsacks can be used to model the $0-1$ linear knapsack sets with uncertain coefficients. In addition to being of theoretical interest, these problems are practically relevant as they can be used to mathematically formulate probabilistic and robust equivalents of the deterministic combinatorial and decision problems.

Although the non-linear binary sets, specifically the quadratic knapsack sets have been studied in the literature, the specific combinatorial structure associated with these sets remains to be explored. Non-linear binary sets involving bilinear terms are at present solved using a combination of lift and project relaxations and a branch-and-bound scheme that solves continuous non-linear relaxations at the nodes of a branch-and-bound search tree. The branch-and-cut methods developed for general integer conic quadratic sets make use of the problem's geometrical structure for removing fractional solutions of conic relaxations can be employed to solve the particular case of $0-1$ conic quadratic knapsacks, however these approaches do not utilize the additional combinatorial structure specific to these sets. Motivated by the performance improvement observed by exploring geometrical structure for conic mixed integer programs, and the fact that exploring combinatorial structure has proven extremely useful in addressing the linear $0-1$ knapsack sets, we expect this to work well in the case of conic quadratic knapsacks as well.

In this dissertation, we study pure-binary programs with conic quadratic constraints and develop branch-and-cut algorithms to solve them with applications to robust network design problem. First, we study the combinatorial structure embedded into these problems with

assumptions of monotonicity and develop valid inequalities for these problems. In Chapter 2, we consider a more general version of the problem without any monotonicity assumptions on the conic constraint, and derive valid inequalities linear in the space of the original variables. These cuts generalize a well-known class of linear cuts for binary knapsacks, and turn out to be very effective in reducing the computational effort involved in solving some practical problems.

In Chapter 3, we propose a further generalization of the problem without any structural assumptions of the constraint in context and study the binary quadratically constrained set. We show that our results generalize several known results for the $0-1$ non-linear constrained sets. We take a detour from combinatorial discussion and develop a geometrical understanding for $0-1$ quadratic problems in Chapter 4. We develop convexifications for the non-convex quadratic sets defined over a hypercube and provide strengthening procedures for the same.

Finally, in Chapter 5, we study the problem of robust network design with uncertainties on the arc capacities. We formulate the robust network design problem as a $0-1$ conic quadratic program without particular assumptions on the characteristics of uncertainties. We consider the scenarios when the uncertainties on the arc capacities are independent and correlated. We show that the inequalities derived prove to be useful in our computational experiments.

Acknowledgments

“ *It is good to have an end to journey toward; but it is the journey that matters, in the end.* ”

Indeed, we can only *connect the dots* looking backwards. It has been quite a while, though it seems like just yesterday that I embarked on this journey which has resulted in and essentially culminates with this dissertation. A journey that has both been academically challenging and personally gratifying. Ever since my arrival at Berkeley, I have been bestowed with love and wisdom of people who I had the biggest fortune of sharing my journey with. People who witnessed every step of it, celebrating with me the joys of reaching milestones, inspiring me through the struggles and believing in me during the moments of self-doubt. This dissertation would not have been remotely possible without their persistent guidance and unconditional support. Even though I am soundly aware that I cannot express my heartfelt gratitude enough, however hard I try; I take this opportunity, nevertheless, to convey my sincerest appreciation for everyone who has made this journey possible for me.

There are only few who are aware of the fact that I almost did not come to Berkeley. In retrospect, it seems almost serendipitous, and it wouldn't have been possible without the efforts of my academic advisor Professor Alper Atamtürk. Alper has been an unabating source of inspiration for me. Throughout my journey as a doctoral student he has found and instilled confidence in me, and mentored me at every step both personally and professionally. His attitude towards research and passion for mathematical rigour is extremely infectious and I have always come out feeling highly invigorated from our countless meetings over all these years. Along with his academic mentorship, I will always be grateful for his solicitude towards my non-academic pursuits. I find myself extremely fortunate and will forever cherish this enriching relationship that I had the fortune of sharing with him.

I have been very fortuitous to have had the opportunity of learning under the tutelage of great scholars. During the first two years of my coursework I took several classes with Professor Ilan Adler. It was his enthusiasm and excitement for the subject matter that rooted my interest in Optimization and propelled me to pursue my doctoral dissertation in this field. My first interaction with Professor Bernd Sturmfels was during Fall of 2010 which was an extremely stimulating experience and helped me appreciate and develop an algebraic geometry perspective for Mathematical Optimization problems. I will always remember my interactions with Professor Phil Kaminsky. Talking to Phil has always been an uplifting experience. Even with his busy schedule and responsibilities as Chair of the department, Phil has always been available, supportive and ever so helpful. I feel overwhelmed to have all of them as members of my dissertation committee. Most of this dissertation can very justly be attributed to their invaluable suggestions and thought-provoking questions.

While the faculty was instrumental in helping me develop an academic penchant, having multifaceted cohorts with interests ranging from creating origamis to discussing chess strategies made the "ungodly hour" discussions at office fun beyond measure. I could not have asked for better fellow group members than Chen, Birce, Qi, Carlos and Andrés. Chen has always been excited about any and every discussion I have had with him, regardless of the topic of discussion. With a passion for research and a drive for mathematical elegance, I have always found him ready for our white-board rundowns. I am also grateful for all the mentors I have had throughout this journey. In particular, I would like to convey my ernest gratitude to Nitish Bahadur, Nguyen Truong, Caitlin Marshall, Vishnu Narayanan and Deepak Rajan for their prudent guidance which has been pivotal during several indecisive junctions.

I consider myself blessed to have been surrounded by friends who have gradually become a second family to me thousands of miles away from home. Friends, who cheered me during my successes, laughed with me when I was happy, embraced me when sad, patiently lent me their ears when I was disconcerted, and their time, irrespective of the hour, when I was struggling. They came together to form a support system that not only would always break the fall when I fell, but also reinvigorated me to go beyond what I thought were my limits. There have been several who I have had the greatest fortune of meeting, acquaintances who left a consequential influence on me during the short sparks of times we spent together. However, there are only a handful who have known me since my very first days in Berkeley. I met Debanjan moments after I arrived in Berkeley, little did I know about what was to follow. I have known Debanjan as a roommate, an academic, a musician but most importantly as a friend who would go out of his way to make sure things are good with me. Having Sharanya as a friend has influenced me in ways more than I can imagine. She has been the quintessential and generous host whenever I reached out to her. She has lent me ears when I needed to vent and she has most graciously obliged whenever I was missing home food. Together with Debanjan, she makes for the two friends whom I have spent the most time with in Berkeley. In Aditya, I found a very special friend with whom I have shared many a laughs and just as well my anxieties and worries. I have known Aditya for eleven years since college, and during all these years he's been the sagacious voice that calms me during the moments of apprehension. I can't forget the hours Anuj and I have spent drinking *adrak wali chai* while discussing matters of earthly importance. Anuj and I have many common academic and non-academic interests, though with a passion for Hindi language we both share a special inclination towards poetry and have spent innumerable hours with our own version of *poetry slam*. He is someone I have always considered to be my partner in crime in whatever I do. With Shachi, I share some of my most happy and indelible memories. Not only we share a fortunate coincidence that we started graduate school together and we finished our doctoral dissertations together, but she has always been ever so excited and actively partaken in my long-distance running endeavors, whether it was my first half-marathon or the ultra distance races. She was my first *pacer* and I can't imagine being the runner and in turn the person I am had it not been for her relentless support during the early days. She has seen the best and the worst of me, and continues to motivate me while I keep trying to push my limits.

There are times when I reminisce about the person I was when I came to Berkeley. The stark contrast between the past and present leaves me perplexed and fascinated at the same time. Most of how much I have grown personally can be attributed to a very special friend I found in Shweta and with whom I got the chance to discover, re-discover and further explore lot of my creative interests. Words are insufficient to express how fortunate I am to have had her as a friend thus far, and her relentless efforts in looking out for me and ensuring my well-being. She simultaneously takes on the part of one of my biggest critics, and one of my strongest supports - and leaves me amazed every time, wondering how she manages to do that. It is with her that I have learnt to adorn successes and failures just the same. As this dissertation comes to an end and nostalgia fills me up, I can't help but reflect on all the adventures we have undertaken together over the years. We have laughed together over anything and everything, be it our most savored obsessions or most dreaded phobias. Although it was serendipitous, it is however unfathomable for me to envisage this journey without her endearing friendship and unrelenting support.

Words fail me every time I try to express my love and thanks for my parents. Pursuing doctoral studies involves remarkable levels of support and patience from one's family. I am forever indebted to my father, mother, and my brother for being there for me and for supporting me from the other end of the the planet. They always had kind words and loving embraces for me. My father and mother have always valued education as the highest priority in an individuals life. They fought against all hardships and made immense sacrifices to make me what I am today. My mother has been my rock all through my life. As a housewife, and more importantly as an air force wife, she has faced a lot of adversities herself but has always shielded me from anything and everything. My father is my idol, he has never let anything hinder my academic and creative pursuits and continued to provide us with top-class resources even with a modest family income. I am thankful that I had such a background to inspire me during the course of my doctoral studies. The true extent of their heroic feat I perhaps will be able to fathom one day. Till then, I will continue to be amazed and astonished at the tremendous support and unconditional love they have showered me with. Trying to grow up would not have been half as much fun had it not been for my little brother being around me and being my partner in crime. He has a determined self-belief, and an infectious energy that has often taught me a thing or two. I am thankful to him for having made such invaluable contributions in constructing a support system for me as I began my doctoral studies thousands of miles away from home. I thank them from the very bottom of my heart, and hope to continue to make them proud in the times to come. This dissertation is dedicated to them.

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norms and reach for the stars. Whether it is the confidence it has instilled in me to question everything, or the courage to fearlessly take on the biggest challenges, or the weather it has spoilt me with, Berkeley has continued to amaze me, inspire me, challenge me, and pamper me through these years, so much so that it has become my second home.

> “*Too many fragments of the spirit have I scattered in these streets, ..and I cannot withdraw from them without a burden and an ache.*”
>
> Kahlil Gibran, *The Prophet*, 1923

To *Ma* and *Pa*

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Chapter 1

Introduction

The aim of this dissertation is to develop new methodologies and algorithms to solve binary conic quadratic programs (BCQPs), which are $0-1$ optimization problems with second order cone constraints. This dissertation consists of four parts. The first part focuses on defining valid inequalities for second-order conic binary programs under structural assumptions of monotonicity. In subsequent chapters, we relax these assumptions in order to develop a generalization of the aforementioned inequalities for second order cone programs and quadratically constrained programs with pure binary variables. Finally, we present an application of the developed solution methodologies in form of a robust network design problem with uncertain arc capacities.

In the last three decades, there have been major advances in our capability of solving linear mixed-integer programming problems. Strong cutting planes obtained through polyhedral analysis of problem structure contributed to this success by strengthening the continuous relaxations of the mixed-integer programs. Powerful cutting planes based on simple substructures of problems are standard features of state-of-the-art optimization software packages, and help a long way in the computational efficiency in solving these problems.

While the 80's and 90's saw the advent in studies of polyhedral structure of linear integer programming, the last decade witnessed conic integer programming receiving particular attention from the mathematical programming community, not only because they are hard to solve and have extremely rich structural properties, but also because of the numerous applications that can be modeled as conic mixed integer programs. Some of these applications are in robust optimization, finance, control theory, and combinatorial optimization. Specifically, the PSD cone (cone of the positive semidefinite matrices) and the second order cone (Lorentz cone) have been the center of attention with respect to the mixed integer conic programming. Most of the research in the theory of cutting plane algorithms and studying polyhedral structure for mixed integer conic programming has been focused on generalizing the ideas from mixed integer linear programming.

A structured variant of these problems arises when the feasible set of the problem is restricted to be a subset of the hypercube. In addition to being of theoretical interest, these problems are practically relevant as they can be used to mathematically formulate probabilistic and robust equivalents of the deterministic combinatorial and decision problems. Uncertainties in data are naturally prevalent in all practical optimization problems, and thus the importance of making decisions under uncertainty cannot be discounted. It is thus of interest to study the probabilistic counterparts of deterministic combinatorial polytopes, in particular exploring the polyhedral structure of binary conic optimization problems and studying their generalizations in form of mixed binary conic optimization problems.

However, the study of solution procedures for BCQPs has not received particular attention. At present, BCQPs are solved using the generic cutting planes developed for mixed integer conic quadratic programs in the branch-and-bound tree, without exploring the underlying combinatorial structure prevailing in such problem. In this dissertation we attempt to address this issue. We develop specific cutting planes that can be incorporated into branch-and-bound solvers for binary conic quadratic problems.

In Chapter 2, we develop valid inequalities for solving BCQPs under structural assumptions which ensure monotonicity of the underlying set functions. While the discussion is motivated by understanding the polyhedral structure of BCQPs, the derived inequalities are valid for a much bigger class of problems with similar combinatorial structure namely *supermodular covering constraints*.

We then relax the monotonicity assumptions for the underlying set functions and study the problem of understanding the polyhedral structure of the general submodular knapsack polytope. In Chapter 3, we show, without any monotonicity assumptions on the underlying set function, that the valid inequalities for this polytope are closely related to the linear $0-1$ knapsack set. In addition, our results directly reduce to the corresponding results for special cases such as linear $0-1$ programs and monotone submodular set functions.

In Chapter 4 we focus our attention to a superclass of BCQPs, i.e. quadratically constrained problems with $0-1$ variables. We provide a geometric understanding of these sets and develop convexifications for the non-convex quadratic sets defined over a hypercube. We also provide a contrast between the geometrical and combinatorial approaches to solve quadratically constrained problems. In Chapter 5 we study an application of the binary conic quadratic programs in form of robust network design problem with uncertain arc capacities. We formulate the robust network design problem as a $0-1$ conic quadratic program without particular assumptions on the characteristics of uncertainties. A row generation approach is proposed with robust minimum cut problem as a separation problem. In the particular case when arc capacities are independent, we exploit the supermodularity of the set functions of the underlying constraints. A reformulation is proposed to recover the supermodularity in case of correlations. Our preliminary computational results indicate that exploring this combinatorial structure of problem provides significant advantages over straightforward use of commercial solvers.

1.1 Notation

We assume that all data is rational throughout this dissertation.

For a finite set N, we use 2^N to denote the set of all subsets of N.

The integers, real numbers, and rational numbers are denoted by $\mathbb{Z}$, $\mathbb{R}$, and $\mathbb{Q}$, respectively. We use $\mathbb{R}_+$ to denote the set of all non-negative real numbers (and similarly for other sets). Given a set N, we use $\mathbb{R}^N$ to denote the set (Euclidean inner-product space) of real vectors whose components are indexed by the elements of N. Given $n \in \mathbb{Z}_+$, we use $\mathbb{R}^n$ to denote $\mathbb{R}^{\{1,\dots,n\}}$. For $x \in \mathbb{R}^N$, we define $x(S) := \sum_{j \in S} x_j$, for $S \subseteq N$. We use similar notation for $\mathbb{Q}^N$, $\mathbb{Z}^N$, etc.

For $\alpha \in \mathbb{R}$, we define $\lfloor \alpha \rfloor := \max\{x \in \mathbb{Z} \ : \ x \le \alpha\}$ and $\lceil \alpha \rceil := \min\{x \in \mathbb{Z} \ : \ x \ge \alpha\}$. Also, we use $(\alpha)^+$ to denote $\max\{\alpha, 0\}$ (the parentheses will be omitted when there is no ambiguity), $\alpha^- := (-\alpha)^+$ and $|\alpha| := \max\{\alpha, -\alpha\}$.

For notational simplicity, we denote a singleton set $\{i\}$ with its unique element i. For a vector $\mathbf{v} \in \mathbb{R}^N$, we use $\mathbf{v}(S)$ to denote $\sum_{i \in S} v_i$ for $S \subseteq N$. For an ordered set $\{s_1, s_2, \dots, s_n\}$, the subset $\{s_i, s_{i+1}, \dots, s_j\} = \emptyset$, $\forall i > j$.

Given a matrix A, we use $A^\top$ to denote its transpose.

1.2 An Overview of Mixed-Integer Programming

A *mixed-integer program* (MIP) is an optimization problem of the form

$$\min \left\{ c^\top x + h^\top y \ : \ (x, y) \in S, (x, y) \in \mathbb{Z}^n \times \mathbb{R}^p \right\} \ , \tag{1.1}$$

where $S \subseteq \mathbb{R}^{n+p}$ is some constraint set, and $c \in \mathbb{R}^n$, $h \in \mathbb{R}^p$. Let $T \subseteq S$ denote the feasible region of (1.1). We may assume that the objective function is linear without any loss of generality: If the objective is $f(x, y)$, we can add an auxiliary variable z and minimize z subject to the original constraints along with $f(x, y) \le z$. If $p = 0$, we call the MIP a *pure integer program* (IP). It is known that unless S is bounded, (1.1) is undecidable [50] for an arbitrary S.

Definition 1.1. Given $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$, the set $H := \left\{x \in \mathbb{R}^n \ : \ a^\top x = b\right\}$ is called an *affine hyperplane*.

Definition 1.2. Given a hyperplane $H = \left\{x \in \mathbb{R}^n \ : \ a^\top x = b\right\} \subseteq \mathbb{R}^n$, the set $\mathbb{R}^n \setminus H$ is the union of two open convex sets called *open halfspaces*: $H_- := \left\{x \in \mathbb{R}^n \ : \ a^\top x < b\right\}$, and $H_+ := \left\{x \in \mathbb{R}^n \ : \ a^\top x > b\right\}$. The closed sets $\overline{H_+} := H_+ \cup H$ and $\overline{H_-} := H_- \cup H$ are called *closed halfspaces*.

Definition 1.3. A polyhedron $P \subseteq \mathbb{R}^n$ is an intersection of a finite number of (closed) halfspaces.

If the set S in (1.1) is polyhedral, we call the MIP a *linear mixed-integer program* (LMIP). See [81], [71], and [97] for a comprehensive study on linear mixed-integer programming.

The feasible region of a mixed-integer program need not be convex. However, we can use a convex set containing the feasible region instead.

Definition 1.4. Given a set $W \subseteq \mathbb{R}^k$ (for a given $k \in \mathbb{Z}_+$), the convex hull of W is defined as the set of all finite convex combinations of points in W. It is denoted by $\mathrm{conv}(W)$.

It is well-known that the convex hull of a set W is the smallest convex set containing W, and is equal to the intersection of all convex sets containing W.

Theorem 1.1. (Theorem I.4.6.3, [71]) *If $T \neq \emptyset$, it follows that*

$$\min \left\{ c^\top x + h^\top y \; : \; (x,y) \in T \right\} = \min \left\{ c^\top x + h^\top y \; : \; (x,y) \in \mathrm{conv}(T) \right\} \; .$$

Definition 1.5. The inequality $f(x,y) \leq \gamma$ is called a *valid inequality* for T if $f(x,y) \leq \gamma$ for all $(x,y) \in T$.

The following definitions are concerned with linear mixed-integer programs, i.e., when S is a polyhedron.

Definition 1.6. Any valid inequality $\pi^\top x + \mu^\top y \leq \pi_0$ for T defines a *face*

$$F := \left\{ (x,y) \in \mathrm{conv}(T) \; : \; \pi^\top x + \mu^\top y = \pi_0 \right\}$$

of $\mathrm{conv}(T)$.

Note that the face of a polyhedron is a polyhedron.

Definition 1.7. A set of points $(x^1, y^1), \ldots, (x^k, y^k)$ is *affinely independent* if $\lambda = 0$ is the unique solution to the set of equations $\sum_{i=1}^k \lambda_i (x^i, y^i) = 0,\ \sum_{i=1}^k \lambda_i = 0$.

Definition 1.8. The dimension of a polyhedron $P \subseteq \mathbb{R}^n$ is k (denoted $\dim(P) = k$) if the maximum number of affinely independent points in P is $k+1$.

Definition 1.9. A face F of a polyhedron P is called a *facet of P* if $\dim(F) = \dim(P) - 1$. Any valid inequality defining F is called a *facet-defining inequality.*

In the polyhedral case, the strength of an inequality is measured by the dimension of the face it defines. An inequality that defines a face of higher dimension is considered to be a stronger inequality. Thus, the strongest valid inequalities for polyhedra are the facet-defining inequalities.

We now present the *Branch-and-Bound* algorithm [58] to solve the MIP (1.1). There are several other approaches to solve MIPs, such as Lagrangian Relaxation, Benders' Decomposition, and Column Generation. We direct the reader to Nemhauser and Wolsey [71] for details of these other methods.

1. (Initialization) Let $\mathcal{L} = \{MIP\}$, $Q^0 = Q$, $\underline{z}^0 = \infty$, and $\bar{z}_{MIP} = \infty$.
2. (Termination test) If $\mathcal{L} = \emptyset$, then the solution (x^0, y^0) with objective $\bar{z}_{MIP} = c^\top x^0 + h^\top y^0$ is optimal. Stop.
3. (Problem selection and relaxation) Select and delete a problem MIP^i from $\mathcal{L}$. Solve its relaxation RP^i to obtain an optimal solution (x^i_R, y^i_R) (if it exists) with objective value z^i_R.
4. (Pruning)
   a) If $z^i_R \geq \bar{z}_{MIP}$, go to Step 2.
   b) If (x^i_R, y^i_R) is infeasible, go to Step 5.
   c) If (x^i_R, y^i_R) is feasible with $z^i_R < \bar{z}_{MIP}$, Let $\bar{z}_{MIP} = z^i_R$. Delete from $\mathcal{L}$ all problems i with $\underline{z}^i \leq \bar{z}_{MIP}$.
5. (Division) Let Q^i be the feasible region of MIP^i and let $\{Q^{ij} : j = 1, \ldots, k\}$ be a division of Q^i. Add problem MIP^{ij} to $\mathcal{L}$ where $\underline{z}^{ij} = z^i_R$ for all $j = 1, \ldots, k$. Go to Step 2.

In practice, the Branch-and-Bound algorithm alone is never used. Instead, a modified form called the *Branch-and-Cut* algorithm is used. In this algorithm, whenever the continuous relaxation is solved, the algorithm checks whether there exists a valid inequality that is violated by the optimal solution (x^i_R, y^i_R) to the relaxation RP^i. In case such an inequality $f(x, y) \leq \gamma$ is found, it is added as an additional constraints to RP^i, and the problem is re-solved, and the algorithm goes back to step 3. If no such inequality is found, the algorithm continues with step 5.

In general, the number of nodes explored by the Branch-and-Bound algorithm is exponential in the input size of the problem. By the addition of valid inequalities as cuts, the lower bound can be improved, and so the number of nodes can be reduced at the cost of the effort taken to compute such cuts. If the extreme point solution to RP^i is fractional, there always exists such a cut (follows from Theorem 1.1 and the Separation Theorem for convex sets). However, in practice, finding such cuts is computationally hard, and the Branch-and-Cut algorithm usually checks whether the relaxation solution violates a certain class of predetermined valid inequalities. Typically, Branch-and-Cut outperforms the Branch-and-Bound algorithm both in terms of computational time and the number of nodes explored.

1.3 Lifting for Linear Mixed-Integer Programming

Lifting refers to the process of extending inequalities that are valid for a restriction S_R of a mixed integer set S to S. Here, we limit our attention to lower dimensional restrictions obtained by fixing variables (usually to their bounds). For a detailed exposure to lifting, we direct the reader to references such as [6, 7, 44, 74, 62, 77, 78, 96, 98].

Consider the feasible region

$$\mathcal{F} := \{x \in \mathbb{R}^m \;:\; Ax \leq b,\ \sum_{j\in S_i} g_j x_j \leq v_i, i = 1,\dots,t\ x_j \in \{0,1\} \text{ for } j \in I\}.$$

Here, $\{S_i\}_{i=1}^{\top}$ is a partition of the set $\{1,\dots,m\}$. Let us fix $x_j = d_j$ for $j \notin S_1$. Let $\mathcal{F}^k = \{x \in \mathbb{R}^{S_1} \;:\; \sum_{m=1}^{k} \sum_{j\in S_m} A_j x_j \leq \bar{b}_k,\ \sum_{j\in S_i} g_j x_j \leq v_i, i = 1,\dots,k\ x_j \in \{0,1\}, j \in I \cap \cup_{m=1}^{k} S_m\}$. Here $\bar{b}_k = b - \sum_{j=k+1}^{\top} A_j d_j$. Suppose we have a valid inequality $\sum_{j\in S_1} \alpha_j x_j \leq \beta$ for conv$(\mathcal{F}^1)$, and we wish to find a valid inequality of the form

$$\sum_{j\in S_1} \alpha_j x_j + \sum_{2\leq k\leq t} \sum_{j\in S_k} \alpha_j (x_j - d_j) \leq \beta \tag{1.2}$$

for conv$(\mathcal{F})$. The problem of finding such an inequality is known as the lifting problem [41]. We introduce all variables in S_k at a time simultaneously into the inequality and sequentially lift in the order $S_2,\dots,S_t$. At stage k, when we have lifted $S_2,\dots,S_{k-1}$, the *lifting function* is defined as

$$\begin{aligned} f_k(z) := \min \quad & \beta - \sum_{j\in S_1} \alpha_j x_j - \sum_{2\leq m<k} \sum_{j\in S_m} \alpha_j (x_j - d_j) \\ \text{s.t.} \quad & \sum_{j\in S_1} \alpha_j x_j + \sum_{2\leq m<k} \alpha_j (x_j - d_j) \;\leq\; \bar{b}_1 - z \\ & \sum_{j\in S_m} g_j x_j \;\leq\; v_m, \quad m = 1,\dots,k-1 \\ & x_j \;\in\; \{0,1\}, \quad j \in I \cap (S_1 \cup \dots \cup S_{k-1}), \end{aligned}$$

where

$$\sum_{j\in S_1} \alpha_j x_j + \sum_{2\leq m<k} \sum_{j\in S_m} \alpha_j (x_j - d_j) \leq \beta \tag{1.3}$$

is valid for conv$(\mathcal{F}^{k-1})$. The corresponding *support function* is

$$\begin{aligned} h_k(z) := \max \quad & \sum_{j\in S_k} \alpha_j (x_j - d_j) \\ \text{s.t.} \quad & \sum_{j\in S_k} A_j (x_j - d_j) \;=\; z \\ & \sum_{j\in S_k} g_j x_j \;\leq\; v_k \\ & x_j \;\in\; \{0,1\}. \quad j \in S_k \cap I. \end{aligned}$$

The following are well known results on lifting.

Theorem 1.2. ([41]) *If we choose α_j, $j \in S_k$ such that $h_k(z) \leq f_k(z)$ for all z, then the lifted inequality* (1.2) *is valid for* $\text{conv}(\mathcal{F}^k)$.

Theorem 1.3. ([41]) *If $h_k(z) = f_k(z)$ has $|S_k|$ solutions $x^1, \dots, x^{|S_k|}$ such that $x^1 - d, \dots, x^{|S_k|} - d$ are linearly independent, and* (1.3) *is facet defining for* $\text{conv}(\mathcal{F}^{k-1})$*, then the lifted inequality* (1.2) *is facet defining for* $\text{conv}(\mathcal{F}^k)$.

For $k = 2, \dots, t$, let Z_k denote the feasible region on which the associated support function $h_k(z)$ attains a finite value. Let Z be a convex set such that $Z_k \subseteq Z$ for all $k = 2, \dots, t$.

Theorem 1.4. ([41]) *Suppose $\tilde{f}$ is a superadditive function on Z, (i.e., $\tilde{f}(z_1) + \tilde{f}(z_2) \leq \tilde{f}(z_1 + z_2)$ for all $z_1, z_2 \in Z$), such that $\tilde{f} \leq f(z)$, then if $\alpha_j, j \in S_k$ are chosen such that $h_k(z) \leq \tilde{f}(z)$ for all $k = 2, \dots, t$, then* (1.2) *is valid for* $\text{conv}(\mathcal{F})$.

1.4 Submodular Functions and Related Polyhedra

In this section, we present some background information on submodular functions and polymatroids that will be used later in this dissertation. Throughout this section, we assume that N is a finite set.

Definition 1.10. A function $f : 2^N \to \mathbb{R}$ is called a *set function on N*.

Definition 1.11. Let f be a set function on N. Then, f is said to be *nondecreasing* if $f(S) \leq f(T)$ for all $S \subseteq T \subseteq N$.

Definition 1.12. Let f be a set function on N. Then, f is said to be *submodular* if $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$ for all $S, T \subseteq N$.

The next theorem gives an alternate characterization for submodular functions.

Theorem 1.5. [80] *Let f be a set function on N. Then, f is submodular if and only if*

$$f(S \cup \{j\}) - f(S) \geq f(S \cup \{j, k\}) - f(S \cup \{k\})$$

for all $S \subseteq N$, $j, k \notin S$, $j \neq k$.

We now introduce two polyhedra associated with submodular functions.

Definition 1.13. Let f be a set function on N. Let

$$EP_f := \left\{ x \in \mathbb{R}^N \ : \ x(S) \leq f(S) \text{ for all } S \subseteq N \right\}.$$

If f is submodular, then EP_f is called the *Extended Polymatroid* associated with f.

Definition 1.14. Let f be a nondecreasing submodular set function on N. Then, the *polymatroid* associated with f is

$$P_f := \left\{ x \in \mathbb{R}_+^N \ : \ x(S) \leq f(S) \text{ for all } S \subseteq N \right\}.$$

Polymatroids have the nice property that the greedy algorithm solves the optimization problem

$$\min \left\{ c^\top x \ : \ x \in P_f \right\}. \tag{1.4}$$

Note that $EP_f \neq \emptyset$ if and only if $f(\emptyset) \geq 0$, and P_f is nonempty if and only if $f(S) \geq 0$ for all $S \subseteq N$. Let $N = \{1, \ldots, n\}$ and let $c_1 \geq \cdots \geq c_k \geq 0 > c_{k+1} \cdots c_n$ for some $k \in N$.

Theorem 1.6. [80] *Let f be a nonnegative submodular set function on N, an optimal solution to* (1.4) *is given by*

$$x_j = \begin{cases} f(S_j) - f(S_j - 1) & \text{for } 1 \leq j \leq k, \\ 0 & \text{for } j > k, \end{cases}$$

where $S_j = \{1, \ldots, j\}$ for $j \in N$, and $S_0 = \emptyset$.

1.5 Applications of Binary Conic Quadratic Programs

In this section, we summarize some of the applications of binary conic quadratic programs. Our prime motivation to study knapsack sets with submodular set functions stems from the need to analyze linear $0-1$ covering constraints with uncertain coefficients. For example, consider the following covering constraint,

$$\boldsymbol{\xi}^\top \mathbf{x} \geq d \tag{1.5}$$

where ξ_i, $i \in \{1, 2, \ldots, N\}$ are random with a support Ξ. Constraint (1.5) does not define a deterministic feasible set. We can approximate the above covering constraint by the following probabilistic constraint,

$$\mathbb{P}(\boldsymbol{\xi}^\top \mathbf{x} \geq d) \geq 1 - \epsilon, \quad \epsilon > 0. \tag{1.6}$$

The probabilistic constraint (1.6), on $x \in \{0, 1\}^N$ with , $0 < \epsilon < 0.5$, can be modeled as a conic quadratic $0-1$ covering knapsack,

$$X_{CQ} := \left\{ \mathbf{x} \in \{0, 1\}^m \ : \ \mathbf{u}^\top \mathbf{x} - \Omega(\epsilon) \parallel \boldsymbol{\Sigma}^{\frac{1}{2}} \mathbf{x} \parallel \geq d \right\} \tag{1.7}$$

where u_e is the nominal value of ξ_e, $\boldsymbol{\Sigma}$ is the covariance matrix, and $\Omega(\epsilon) > 0$ is the scaling factor. The term $\Omega(\epsilon) \parallel \boldsymbol{\Sigma} \mathbf{x} \parallel$ is used to build sufficient slack into the constraint to accommodate the variability of ξ_i around the nominal value u_i. Indeed, if ξ_i's are normally distributed independent random variables, then letting u_i and σ_{ii} be the mean and standard deviation of ξ_i, $0 \leq i \leq m$, and $\Omega(\epsilon) = -\varphi^{-1}(\epsilon)$ with $0 < \epsilon < 0.5$, where φ is the standard normal cumulative distribution function, the set of $0-1$ solutions for the probabilistic covering constraint (1.6) is exactly X_{CQ} [31]. On the other hand, if ξ_i's are known only through their first two moments u_i and σ_{ii}^2, then any point in X_{CQ} with $\Omega(\epsilon) = \sqrt{(1-\epsilon)/\epsilon}$ satisfies the probabilistic constraint (1.6) [24, 37]. Alternatively, if ξ_i's are only known to be symmetric with support $[u_i - \sigma_{ii}, u_i + \sigma_{ii}]$, then points in X_{CQ} with $\Omega(\epsilon) = \sqrt{\ln(1/\epsilon)}$ satisfy constraint (1.6) [23, 22]. Hence, under different assumptions of uncertainty on $\boldsymbol{\xi}$, one arrives at different instances of the conic quadratic knapsack set X_{CQ}.

There are several important applications of BCQPs that can be modeled in the aforementioned framework of incorporating uncertainty. Despite the similarities in the structures of the systems, the applications all have different objectives and concerns. Pinar [76] describes a pricing problem for an American option in a financial market under uncertainty. Hijazi et al. [47] investigate a telecommunications network problem that seeks to minimize the network response time to a user request. Mak et al. [63] consider the problem of creating a network infrastructure and providing coverage for battery swapping stations to service electric vehicles. The number of electric vehicles that travel along a path (portion of a path) is random, so demand at each swapping station is uncertain.

In addition to being of theoretical interest, binary conic-quadratic programming problems are practically relevant as they can be used to mathematically formulate probabilistic and robust equivalents of the deterministic combinatorial and decision problems. Uncertainties in data are naturally prevalent in all practical optimization problems, and thus the importance of making decisions under uncertainty cannot be discounted.

1.6 Solution Approaches for Binary Conic Quadratic Programs

A popular approach for linearization of bilinearities occuring in the binary (conic) quadratic knapsacks is due to McCormick. McCormick [66] proposes to relax the set

$$B = \{(x_1, x_2, z) \in [0,1] \times [0,1] \times \mathbb{R} \ : \ z = x_1 x_2\}$$

with the following inequalities, which we refer to as the *McCormick inequalities*:

$$z \geq \max(x_1 + x_2 - 1, 0), \qquad z \leq \min(x_1, x_2) \tag{1.8}$$

Al-Khayyal and Falk [54] show that the convex hull of B is described by the McCormick inequalities. Padberg [73] studies the Boolean Quadric Polytope associated with the bilinearities and derives facet defining inequalities for the same. This however is a theoretical work and these inequalities have not been used in literature for computational analysis.

Clearly, any method for general nonlinear integer programming applies to conic integer programming. Sherali and Adams [82] generalize the idea of McCormick as Reformulation-Linearization Technique (RLT). Initially developed for linear $0-1$ programming, RLT has been extended to nonconvex optimization problems [86]. Stubbs and Mehrotra [87, 88] generalize the lift-and-project method [16] of Balas et al. for $0-1$ mixed convex programming. See also Balas [14] and Sherali and Shetti [84] on disjunctive programming methods. Kojima and Tunçel [57] give successive semidefinite relaxations converging to the convex hull of a nonconvex set defined by quadratic functions. These relaxations can be used to model second order conic mixed $0-1$ programs as follows. The second order conic constraints can be written as nonconvex quadratic constraints. For the binary variables $x_j,\ j \in N$, we can add the nonconvex quadratic equality constraint $x_j - x_j^2 = 0$. Lasserre [59] describes a hierarchy of semidefinite relaxations of nonlinear $0-1$ programs.

Common to all of these above general approaches is a hierarchy of convex relaxations in higher dimensional spaces whose size grows exponentially with the size of the original formulation. Therefore, using such convex relaxations in higher dimensions is impractical except for very small instances. On the other hand, projecting these formulations to the original space of variables is also difficult except for certain special cases.

Another stream of research is the development of branch-and-bound algorithms for nonlinear integer programming based on linear outer approximations [2, 91, 21, 93]. Duran and Grossmann [35] in their seminal work develop the idea of deriving polyhedral approximations of mixed integer non-linear programs (linear in integer variables) by solving an alternating finite sequence of nonlinear programming subproblems and relax versions of a mixed-integer linear master program. Fletcher and Leyffer [39] discuss non-differentiable functions in the context of outer approximation approaches for MINLP, where the authors prove convergence of outer approximation algorithms for nonsmooth penalty functions. The only article dealing with outer approximation techniques for MISOCPs is by Vielma et al. [93], which is based on Ben-Tal and Nemirovski's polyhedral approximation of the second order cone constraints [21]. Drewes and Ulrich [34] present a hybrid branch and bound based outer approximation scheme for MISOCPs, where the entire outer approximation is not chosen in advance, however is strengthened iteratively in order to guarantee convergence of the algorithm. The proposed idea is to iteratively compute integer feasible solutions of a subgradient based linear outer approximation of a MISOCP and to tighten this outer approximation by solving nonlinear continuous problems. The advantage of linear approximations is that they can be solved fast; however, the bounds from linear approximations may not be strong. In the case of conic programming, and in particular second-order cone programming, existence of efficient algorithms permits the use of continuous conic relaxations at the nodes of the branch-and-bound tree, although the lack of effective warm-starts is a significant disadvantage.

One of the first studies on developing valid inequalities for conic integer sets directly is due to Çezik and Iyengar [30]. They study techniques for generating valid convex constraints for mixed 0-1 conic programs and show that many of the techniques developed for generating linear cuts for linear mixed 0-1 optimization, such as the Gomory cuts, the lift-and-project cuts, and cuts from other hierarchies of tighter relaxations, extend to conic mixed 0-1 optimization. Atamtürk and Narayanan [9] describe a general mixed-integer rounding approach for conic quadratic mixed-integer sets. Their approach for deriving valid inequalities for SOCMIP is to reformulate second-order conic constraints in a higher dimensional space that leads to a natural decomposition into simpler polyhedral sets and to analyze each of these sets. Atamtürk and Narayanan [10] describe lifting techniques for conic discrete optimization. Belotti et al. [19] give conic cuts for conic quadratic integer optimization. Anderson and Jensen [4] give intersection cuts for conic quadratic mixed-integer sets. Kilinç-Karzan [55] describes minimal inequalities for conic mixed-integer programs. Modaresi et al. [67] give split cuts and extended formulations for conic quadratic mixed-integer programming. Kilinç-Karzan and Yildiz [56] describe two-term disjunction inequalities for the second-order cone.

These aforementioned works however are on general conic quadratic discrete optimization and do not exploit any special structure specifically the combinatorial structure associated with the problem studied here.

1.7 Final Remarks

From the previous sections, we see that although Binary Conic Quadratic Programs have several applications in important problems, the current state of solution technologies do not exploit any specific structure related to these problems. Solution approaches including deriving strong valid inequalities that have earlier been developed for linear programming have been generalized to conic optimization problems. We also have readily available open source software for continuous conic optimization, e.g., CSDP[27], DSDP[20], SDPA[99], SDPT3[92], SeDuMi[89]. Commercial software vendors, e.g., ILOG and MOSEK, have responded to the demand for solving (continuous) conic optimization problems by including solvers for second-order cone programming (SOCP) in their recent versions.

We attempt to make use of these above developments to study the combinatorial structure of these problems and improve the computational effort involved in solving Binary Conic Quadratic Programs, by designing strong valid inequalities that can be used at the nodes of the Branch-and-Bound tree to cut off fractional solutions. Our attention is restricted to those classes of inequalities that can be easily incorporated in the above mentioned solvers (i.e., linear and conic inequalities).

Chapter 2

Supermodular Covering Knapsack Polytope

2.1 Introduction

Our main motivation for studying the supermodular covering knapsack set is to address linear 0-1 covering constraints with uncertain coefficients. If the coefficients $\tilde{u}_i$, $i \in N$, of the constraint are random variables, then a probabilistic (chance) constraint

$$\mathbb{P}(\tilde{\mathbf{u}}^\top \mathbf{x} \geq d) \geq 1 - \epsilon \tag{2.1}$$

on $x \in \{0,1\}^N$ with , $0 < \epsilon < 0.5$, can be modeled as a conic quadratic 0-1 covering knapsack

$$K_{CQ} := \left\{ \ x \in \{0,1\}^N : \mathbf{u}^\top \mathbf{x} \ - \Omega \parallel \mathbf{D}\mathbf{x} \parallel \geq d \ \right\},$$

where u_i is a nominal value and d_i is a deviation statistic for $\tilde{u}_i$, $i \in N$, $\mathbf{D} = \text{diag}(d_1, d_2, \ldots, d_{|N|})$, $\Omega > 0$. Now, consider $f : 2^N \to R$ defined as

$$f(S) = \mathbf{u}(S) - g(\mathbf{c}(S)), \tag{2.2}$$

where $g : \mathbb{R} \to \mathbb{R}$ is a concave function and $\mathbf{u}, \mathbf{c} \in \mathbb{R}^N$. It is easily checked that if $\mathbf{c} \geq \mathbf{0}$, then f is supermodular on N (e.g. Ahmed and Atamtürk [3]). Letting $c_i = \Omega^2 d_i^2$ for $i \in N$, we see that

$$f(S) = \mathbf{u}(S) - \sqrt{\mathbf{c}(S)} \geq d \tag{2.3}$$

if and only if $\chi_S \in K_{CQ}$. Moreover, f is non-decreasing if $u_i \geq \Omega d_i$ for $i \in N$.

Although the polyhedral results in this chapter are for the more general supermodular covering knapsack polytope conv(K), we give examples and a separation algorithm for a specific set function of form (2.2). Because K reduces to the linear $0-1$ covering knapsack set when f is modular, optimization over K is $\mathcal{NP}$-hard.

For a set function f on N and $i \in N$, let its difference function be

$$\rho_i(S) := f(S \cup i) - f(S) \text{ for } S \subseteq N \setminus i.$$

Note that f is supermodular if and only if $\rho_i(S) \leq \rho_i(T), \ \forall S \subseteq T \subseteq N \setminus i$ and $i \in N$; that is, the difference function ρ_i is non-decreasing on $N \setminus i$ (e.g. Schrijver [80]). Furthermore, f is non-decreasing on N if and only if $\rho_i(\cdot) \geq 0$ for all $i \in N$.

2.1.1 Relevant Literature

In a closely related work, Atamtürk and Narayanan [12] study the lower level set of a non-decreasing submodular function. Negating inequality (2.3) yields a knapsack set with non-increasing submodular function $-f$, and, therefore, their results are not applicable here. Indeed, as the upper level set of a non-decreasing supermodular function is equivalent to the lower level set of a non-increasing submodular function, this chapter closes a gap by covering the case complementary to the one treated in Atamtürk and Narayanan [12].

Although there is a rich body of literature in approximation algorithms for submodular or supermodular functions, polyhedral results are scarce. Nemhauser et al. [72], Sviridenko [90], Iwata [49], Lee et al. [60] give approximation algorithms for optimizing submodular/supermodular functions over various constraints. There is an extensive literature on the polyhedral analysis of the linear knapsack set. The polyhedral analysis of the linear knapsack set was initiated by Balas [15], Hammer et al. [45], and Wolsey [95]. For a recent review of the polyhedral results on the linear knapsack set we refer the reader to Atamtürk [6, 5]. Martello and Toth [65] present a survey of solution procedures for linear knapsack problems. Covering knapsack has also been extensively studied in the purview of approximation algorithms and heuristics [33, 26]. Carnes and Shmoys [29] study the flow cover inequalities (Aardal, Pochet and Wolsey [1]) in the context of the deterministic minimum knapsack problem. The majority of the research on the nonlinear knapsack problem is devoted to the case with separable nonlinear functions (Morin [68]). Hochbaum [48] maximizes a separable concave objective function, subject to a packing constraint. There are fewer studies on the nonseparable knapsack problem, most notably on the knapsack problem with quadratic objective and linear constraint. Helmberg et al. [46] give semidefinite programming relaxations of knapsack problems with quadratic objective. Ahmed and Atamtürk [3] consider maximizing a submodular function over a linear knapsack constraint. We refer the reader to also Bretthauer et al. [28], Kellerer [52] for a survey of nonlinear knapsack problems.

The rest of the chapter is organized as follows: Section 2.2 describes the main polyhedral results. It includes pack inequalities, their extensions and lifting. The lifting problems of the pack inequalities are themselves optimization problems over supermodular covering knapsack sets. We derive sequence-independent upper bounds and lower bounds on the lifting coefficients. In Section 2.3 we give a separation algorithm for the pack inequalities for the conic quadratic case. In Section 2.4 we present a computational study on using the results for solving 0-1 optimization problems with conic quadratic constraints.

2.2 Polyhedral Analysis

In this section we analyze the facial structure of the supermodular knapsack covering polytope. In particular, we introduce the pack inequalities and discuss their extensions and lifting. Throughout the rest of this chapter we make the following assumptions:

(**A**.1) f is non-decreasing,

(**A**.2) $f(\emptyset) = 0$,

(**A**.3) $f(N \setminus i) \geq d$ for all $i \in N$.

Because f is supermodular, assumption (**A**.1) is equivalent to $\rho_i(\emptyset) \geq 0, \ \forall\, i \in N$, which can be checked easily. Assumption (**A**.1) holds, for instance, for a function f of the form (2.3) if $u_i \geq \Omega d_i, \forall\, i \in N$. Assumption (**A**.2) can be made without loss of generality as f can be translated otherwise. Finally, if (**A**.3) doesn't hold, i.e., $\exists\, i \in N : f(N \setminus i) < d$, then x_i equals one in every feasible solution.

Proposition 2.1. conv(K) *is a full-dimensional polytope.*

Proof. Define $\mathbb{1}$ to be an n-dimensional vector of ones. From Assumptions (**A**.1) and (**A**.3) it can be seen that the points $\mathbb{1} - e_i$, $i \in N$ along with $\mathbb{1}$ belong to the set K and constitute a set of $n+1$ affinely independent points in K. The result follows. □

Proposition 2.2. *Inequality $x_i \leq 1$, $i \in N$, is facet-defining for* conv(K).

Proof. The points $\mathbb{1}$ and $\mathbb{1} - e_j$, $j \in N \setminus \{i\}$ constitute a set of n affinely independent points satisfying $x_i = 1$. □

Proposition 2.3. *Inequality $x_i \geq 0$, $i \in N$, is facet-defining for* conv(K) *if and only if $f(N \setminus \{i, j\}) \geq d$, $\forall\, j \in N \setminus \{i\}$.*

Proof. If $f(N \setminus \{i, j\}) \geq d, \forall\, j \in N \setminus \{i\}$, then $\mathbb{1} - e_i$ and $\mathbb{1} - e_i - e_j$, $j \in N \setminus \{i\}$ constitute a set of n affinely independent points satisfying $x_i = 0$. Conversely, if $f(N \setminus \{i, j\}) < d$, for some $j \in N \setminus \{i\}$ then

$$\{\mathbf{x} \in K \ : \ x_i = 0\} = \{\mathbf{x} \in K \ : \ x_i = 0, \, x_j = 1\}\,.$$

which cannot have a dimension more than $n - 2$. Hence $x_i \geq 0$ is not facet-defining for conv(K). □

We refer to the facets defined in Propositions 2.2–2.3 as the *trivial facets* of conv(K).

Proposition 2.4. *If inequality* $\sum_{j \in N} \pi_j x_j \geq \pi_0$ *defines a non-trivial facet of* $\text{conv}(K)$*, then* $\pi_0 > 0$ *and* $0 \leq \pi_j \leq \pi_0$*,* $\forall\, j \in N$*.*

Proof. Assume that the inequality $\sum_{j \in N} \pi_j x_j \geq \pi_0$ defines a facet of $\text{conv}(K)$. Now consider a point $\mathbf{x}^* \in K$ such that $\sum_{j \in N} \pi_j x_j^* = \pi_0$ (such a point exists). Without loss of generality assume the aforementioned inequality is different from $x_j \leq 1$, we can assume that $x_j^* < 1$. Since $\text{conv}(K)$ is full dimensional, the point $\bar{\mathbf{x}} = \mathbf{x}^* + \epsilon e_j \in K$ for sufficiently small $\epsilon > 0$. This yields, $\sum_{j \in N} \pi_j \bar{x}_j = \sum_{j \in N} \pi_j x_j^* + \epsilon \pi_j = \pi_0 + \epsilon \pi_j \geq \pi_0$, implying $\pi_j \geq 0, \forall\, j \in N$.

Reconsider the point $\mathbf{x}^*$ on the facet $\sum_{j \in N} \pi_j x_j^* = \pi_0$. Since $\mathbf{x}^* = \mathbf{0} \notin K$ and $\boldsymbol{\pi} \neq 0$, it can be seen that $\pi_0 > 0$. For the last part assume $\exists\, j \in N$ such that $\pi_j > \pi_0$. This implies that $e_j \in K$ and hence the inequality $\sum_{k \in N \setminus j} \pi_k x_k + \pi_0 x_j \geq \pi_0$ is also valid for $\text{conv}(K)$. However this inequality dominates the original inequality which is a contradiction to our assumption that the original inequality defines a facet of $\text{conv}(K)$. $\square$

2.2.1 Pack Inequalities

In this section we define the first class of valid inequalities for K.

Definition 2.1. A subset P of N is a *pack* for K if $\delta := d - f(P) > 0$. A pack P is maximal if $f(P \cup i) \geq d, \;\; \forall\, i \in N \setminus P$.

For a pack $P \subseteq N$ for K, let us define the corresponding *pack inequality* as

$$\mathbf{x}(N \setminus P) \geq 1. \tag{2.4}$$

The pack inequality simply states that at least one element outside the pack P has to be picked to satisfy the knapsack cover constraint $f(\mathbf{x}) \geq d$. Consider the non-empty restriction $K(P) = \{\mathbf{x} \in K : x_i = 1, \forall\, i \in P\}$ of K.

Proposition 2.5. *If* $P \subseteq N$ *is a pack for* K*, then the pack inequality* (2.4) *is valid for* K*. Moreover, it defines a facet of* $\text{conv}(K(P))$ *iff* P *is a maximal pack.*

Proof. Define $\overline{K} := \big\{\mathbf{x} \in \{0,1\}^N \;:\; \mathbf{x}(N \setminus P) < 1\big\}$. It is sufficient to show that $f(\mathbf{x}) < d$ for all $\mathbf{x} \in \overline{K}$. Since $\forall \mathbf{x} \in \overline{K}$, we have $\mathbf{x}(N \setminus P) = 0$, implying $\mathbf{x} \leq \mathbf{y}$, $\forall \mathbf{x} \in \overline{K}$, and $\forall \mathbf{y} \in K(P)$; implying

$$f(\mathbf{x}) \leq f(P) < d,$$

where the first inequality follows from assumption ($\mathbf{A}$.1), that f is non-decreasing.

For the second part, consider the $|N \setminus P|$ points

$$\mathbf{x}^k \in \{0,1\}^N \quad \text{such that} \;\; x_j^k = \begin{cases} 1 & \text{if } j \in P \cup k, \\ 0 & \text{if } j \in N \setminus \{P \cup k\} \end{cases}, \; \forall\, k \,\in\, N \setminus P. \tag{2.5}$$

Since f is non-decreasing and P is a maximal pack, we have $\mathbf{x}^k \in K, \forall\, k \in N \setminus P$. The $|N \setminus P|$ points $\mathbf{x}^k$, $k \in N \setminus P$ are in $\operatorname{conv}(K(P))$ and satisfy (2.4) as equality. It is easily seen that these $|N \setminus P|$ points are linearly independent. Hence for a maximal pack P, (2.4) defines a facet of $\operatorname{conv}(K(P))$.

Conversely suppose that pack P is not maximal. Thus, $\exists\, i \in N \setminus P$ such that $f(P \cup i) < d$. Then the corresponding valid pack inequality

$$\mathbf{x}(N \setminus (P \cup i)) \geq 1$$

and $x_i \geq 0$ dominate (2.4). $\square$

Example 2.1. Consider the conic-quadratic covering knapsack set

$$K = \left\{ \mathbf{x} \in \{0,1\}^4 \ : \ x_1 + 2.5x_2 + 3x_3 + 3x_4 - \sqrt{x_3^2 + x_4^2} \geq 5.5 \right\}.$$

The maximal packs for K and the corresponding pack inequalities are

$$\begin{array}{llllll} \{1,2\}: & x_3 + x_4 \geq 1 & \{1,3\}: & x_2 + x_4 \geq 1 & \{1,4\}: & x_2 + x_3 \geq 1 \\ \{2,3\}: & x_1 + x_4 \geq 1 & \{2,4\}: & x_1 + x_3 \geq 1 & \{3,4\}: & x_1 + x_2 \geq 1. \end{array}$$

It is of interest to note that the pack inequalities derived above require only that f be non-decreasing. Following result proves the validity of pack inequalities in a special case when the covariance matrix $\mathbf{\Sigma}$ is not necessary diagonal.

Proposition 2.6. *The set function $f : \{0,1\}^{|N|} \mapsto \mathbb{R}$ defined as,*

$$f \ := \ \mathbf{u}^\top \mathbf{x} - \sqrt{\mathbf{x}^\top \mathbf{\Sigma} \mathbf{x}}$$

is non-decreasing on N if $u_i \geq \sqrt{2}\,\Omega\,\sigma_i$, $\forall\, i \in N$ and $\mathbf{\Sigma}$ is diagonally dominant, i.e. $\sigma_i^2 \geq \sum_{j \in N \setminus i} |\sigma_{ij}|\ \forall\, i \in N$.

Proof. Consider the following (wlog) for $i \in N$, $S \subseteq N \setminus i$,

$$\begin{aligned} \rho_i(S) &= f(S \cup i) - f(S) \\ &= u_i - \Omega \left(\sqrt{\sum_{j \in S \cup i} \left(\sigma_j^2 + \sum_{k \in S \cup i \setminus j} \sigma_{kj} \right)} - \sqrt{\sum_{j \in S} \left(\sigma_j^2 + \sum_{k \in S \setminus j} \sigma_{kj} \right)} \right) \\ &\geq u_i - \Omega \left(\sqrt{\sigma_i^2 + \sum_{j \in S} \sigma_{ij}} \right) \\ &\geq u_i - \sqrt{2}\,\Omega\,\sigma_i \\ &\geq 0 \end{aligned}$$

where the first inequality follows from the triangle inequality (for $a, b, c \geq 0$, s.t. $a^2 = b^2 + c^2$, then $a \leq b + c$), the second inequality follows from diagonal dominance of $\mathbf{\Sigma}$ and the final inequality follows from the assumption $u_i \geq \sqrt{2}\,\Omega\,\sigma_i,\ \forall\, i \in N$. □

2.2.2 Extended Pack Inequalities

The pack inequalities (2.4), typically, do not define facets of conv(K); however, they can be strengthened by extending them with the elements of the pack. Though unlike in the linear case, for the supermodular covering knapsack set, even simple extensions are sequence-dependent. Proposition 2.7 describes such an extension of the pack inequalities (2.4).

Definition 2.2. Let $P \subseteq N$ be a pack and $\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots, \pi_{|P|})$ be a permutation of the elements of P. Define $P_i := P \setminus \{\pi_1, \pi_2, \ldots, \pi_i\}$ for $i = 1, \ldots, |P|$ with $P_0 = P$. The *reduction* of P with respect to $\boldsymbol{\pi}$ is defined as $R_{\boldsymbol{\pi}}(P) := P \setminus U_{\boldsymbol{\pi}}(P)$, where

$$U_{\boldsymbol{\pi}}(P) := \left\{ \pi_j \in P \ : \ \max_{i \in N \setminus P} \rho_i(N \setminus i) \leq \rho_{\pi_j}(P_j) \right\}. \tag{2.6}$$

For a given pack P and reduction $R_{\boldsymbol{\pi}}(P) = P \setminus U_{\boldsymbol{\pi}}(P)$, we define the *extended pack inequality* as

$$\mathbf{x}(N \setminus R_{\boldsymbol{\pi}}(P)) \geq |U_{\boldsymbol{\pi}}(P)| + 1. \tag{2.7}$$

Proposition 2.7. *If $P \subseteq N$ is a pack for K and $U_{\boldsymbol{\pi}}(P)$ is defined as in* (2.6)*, then the extended pack inequality* (2.7) *is valid for K.*

Proof. Let $L \subseteq N \setminus R_{\boldsymbol{\pi}}(P)$ with $|L| \leq |U_{\boldsymbol{\pi}}(P)|$. To prove the validity of (2.7) it suffices to show that $f(R_{\boldsymbol{\pi}}(P) \cup L) < d$. Let $J = U_{\boldsymbol{\pi}}(P) \setminus L =: \{j_1, j_2, \ldots, j_{|J|}\}$ be indexed consistently with π. Note that for $Q = U_{\boldsymbol{\pi}}(P) \cap L$, we have $|L \setminus Q| \leq |J|$. Then

$$\begin{aligned}
f(R_{\boldsymbol{\pi}}(P) \cup L) &= f(R_{\boldsymbol{\pi}}(P) \cup Q) + \rho_{L \setminus Q}(R_{\boldsymbol{\pi}}(P) \cup Q) \\
&\leq f(R_{\boldsymbol{\pi}}(P) \cup Q) + \sum_{\ell \in L \setminus Q} \rho_\ell(N \setminus \ell) \\
&\leq f(R_{\boldsymbol{\pi}}(P) \cup Q) + \sum_{\pi_j \in J} \rho_{\pi_j}(P_j) \\
&\leq f(R_{\boldsymbol{\pi}}(P) \cup Q) + \sum_{j_i \in J} \rho_{j_i}\left(R_{\boldsymbol{\pi}}(P) \cup Q \cup \{j_{i+1}, \ldots, j_{|J|}\}\right) \\
&= f(P) < d,
\end{aligned}$$

where the first and third inequalities follow from supermodularity of f and the second one from (2.6), $|L \setminus Q| \leq |J|$, and (**A**.1). □

We now provide a sufficient condition for the extended pack inequality to be facet-defining for $\mathrm{conv}(K(R_{\boldsymbol{\pi}}(P)))$.

Proposition 2.8. *The extended pack inequality* (2.7) *is facet-defining for* $\mathrm{conv}(K(R_{\boldsymbol{\pi}}(P)))$ *if P is a maximal pack and for each $i \in U_{\boldsymbol{\pi}}(P)$ there exist distinct $j_i, k_i \in N \setminus P$ such that $f(P \cup \{j_i, k_i\} \setminus i) \geq d$.*

Proof. Consider the points $\chi_{P \cup i}$, $\forall i \in N \setminus P$ and $\chi_{P \cup \{j_i,k_i\} \setminus i}$, $\forall i \in U_{\boldsymbol{\pi}}(P)$ and $j_i, k_i \in N \setminus P$, which are on the face defined by (2.7). The proof will be completed by showing that these $|N \setminus P| + |U_{\boldsymbol{\pi}}(P)|$ points are linearly independent. Let M be the matrix containing these points as rows. Observe that M can be represented as

$$M = \begin{pmatrix} \mathbb{1}_{n \times m} & \mathrm{Id}_n \\ \mathbb{1}_{m \times m} - \mathrm{Id}_m & \mathrm{H}_{m \times n} \end{pmatrix}$$

where $n = |N \setminus P|$ and $m = |U_{\boldsymbol{\pi}}(P)|$. Here $\mathbb{1}_{n \times m}$ denotes an $n \times m$ matrix all of whose entries are 1. Id_n refers to the $n \times n$ identity matrix and $\mathrm{H}_{m \times n}$ is an $m \times n$ binary matrix ($H_{ij} \in \{0,1\}$, $1 \leq i \leq m$, $1 \leq j \leq n$) such that all of its rows sum to two $\left(\sum_{j=1}^{n} H_{ij} = 2, \forall 1 \leq i \leq m\right)$. Now, M is non-singular if and only of

$$M \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = \mathbf{0} \quad \Rightarrow \quad \boldsymbol{\alpha}, \boldsymbol{\beta} = \mathbf{0}, \tag{2.8}$$

where $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are vectors of length of m and n, respectively. The solutions to (2.8) thus satisfy

$$\mathbb{1}_{n \times m}\boldsymbol{\alpha} + \boldsymbol{\beta} = \mathbf{0}, \tag{2.9}$$

$$(\mathbb{1}_{m \times m} - \mathrm{Id}_m)\boldsymbol{\alpha} + \mathrm{H}_{m \times n}\boldsymbol{\beta} = \mathbf{0}. \tag{2.10}$$

Substituting for $\boldsymbol{\beta}$, in (2.10) from (2.9) yields

$$\begin{aligned} (\mathbb{1}_{m \times m} - \mathrm{Id}_m)\boldsymbol{\alpha} - \mathrm{H}_{m \times n}\mathbb{1}_{n \times m}\boldsymbol{\alpha} &= \mathbf{0} \\ (\mathbb{1}_{m \times m} - \mathrm{Id}_m)\boldsymbol{\alpha} - 2\mathbb{1}_{m \times m}\boldsymbol{\alpha} &= \mathbf{0} \\ (\mathbb{1}_{m \times m} + \mathrm{Id}_m)\boldsymbol{\alpha} &= \mathbf{0}. \end{aligned}$$

Thus the problem of proving non-singularity of M boils down to proving non-singularity of $\mathbb{1}_{m \times m} + \mathrm{Id}_m$. To see that $\mathbb{1}_{m \times m} + \mathrm{Id}_m$ is non-singular, consider the following claim.

Claim 2.1. $\boldsymbol{det}(\mathbb{1}_{m \times m} + \mathrm{Id}_m) = m + 1$

Proof. (Proof by Induction): Let $D(m) = \mathbf{det}(\mathbb{1}_{m \times m} + \mathrm{Id}_m)$.

Initial/Base Step: $D(1) = \mathbf{det}(1 + 1) = 2 = 1 + 1$.

Now, assume $D(m) = m + 1$, $\forall\, 1 \le k \le m$

$$\textbf{Inductive Step:} \quad \mathbb{1}_{(m+1)\times(m+1)} + \mathrm{Id}_{m+1} = \begin{pmatrix} 2 & 1 & \cdots & 1 \\ 1 & 2 & \cdots & 1 \\ \vdots & \ddots & & \\ 1 & 1 & \cdots & 2 \end{pmatrix}_{m\times m}$$

$$D(m+1) = 2D(m) - m * \mathbf{det} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 2 & \cdots & 1 \\ \vdots & \ddots & & \\ 1 & 1 & \cdots & 2 \end{pmatrix}_{(m-1)\times(m-1)}$$

$$D(m+1) = 2D(m) - m * 1^*$$

$$D(m+1) = 2(m+1) - m = (m+1) + 1.$$

□

The proof is now complete. □

Example 2.2. (cont.) Consider the conic-quadratic covering knapsack set in the previous example:

$$K = \left\{ \mathbf{x} \in \{0,1\}^4 \ : \ x_1 + 2.5x_2 + 3x_3 + 3x_4 - \sqrt{x_3^2 + x_4^2} \ge 5.5 \right\}.$$

For the maximal pack $P = \{3, 4\}$, we gave the corresponding pack inequality

$$x_1 + x_2 \ge 1.$$

For permutation $\boldsymbol{\pi} = (3, 4)$, $P_1 = \{4\}$ and $P_2 = \emptyset$. As $\rho_3(P_1) = 4 - \sqrt{2} \approx 2.586$ and $\rho_1(\{2, 3, 4\}) = 1$, $\rho_2(\{1, 3, 4\}) = 2.5$, the corresponding reduction $R_{(3,4)}(P) = \{4\}$ gives the extended pack inequality

$$x_1 + x_2 + x_3 \ge 2. \tag{2.11}$$

Alternatively, $\boldsymbol{\pi} = (4, 3)$ yields the reduction $R_{(4,3)}(P) = \{3\}$ and the corresponding extended pack inequality

$$x_1 + x_2 + x_4 \ge 2. \tag{2.12}$$

Observe that inequalities (2.11) and (2.12) are the non-trivial facets of $\mathrm{conv}(K(4))$ and $\mathrm{conv}(K(3))$, respectively.

$$^*\mathbf{det} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1+n & \cdots & 1 \\ \vdots & \ddots & & \\ 1 & 1 & \cdots & 1+n \end{pmatrix}_{m\times m} = n^{m-1} \ \textit{(c.f. Muir, T., 1960)}$$

2.2.3 Lifted Pack Inequalities

In this section we study the lifting problem of the pack inequalities in order to strengthen them. Lifting has been very effective in strengthening inequalities for the linear $0-1$ knapsack set [15, 17, 18, 42, 45, 95]. The lifting problem for the pack inequalities for K is itself an optimization problem over the supermodular covering knapsack set.

Precisely, we lift the pack inequality (2.4) to a valid inequality of the form

$$x(N \setminus P) - \sum_{i \in P} \alpha_i(1 - x_i) \geq 1. \tag{2.13}$$

The lifting coefficients α_i, $i \in P$ can be computed iteratively in some sequence: Suppose the pack inequality (2.4) is lifted with variables x_i, $i \in J \subseteq P$ to obtain the intermediate valid inequality

$$x(N \setminus P) - \sum_{i \in J} \alpha_i(1 - x_i) \geq 1 \tag{2.14}$$

in some sequence of J, then x_k, $k \in P \setminus J$, can be introduced to (2.14) by computing

$$\alpha_k = \varphi(I, k) - 1 - \boldsymbol{\alpha}(J), \tag{2.15}$$

where $\varphi(I, k)$ is the optimal objective value of the following lifting problem, $L(I, k)$:

$$\varphi(I, k) := \min_{T \subseteq I} \left\{ |(N \setminus P) \cap T| + \sum_{i \in J \cap T} \alpha_i \ : \ f(T \cup P \setminus (J \cup k)) \geq d \right\} \tag{2.16}$$

and

$$I = (N \setminus P) \cup J.$$

The lifting coefficients are typically a function of the sequence used for lifting. The extension given in Proposition (2.7) may be seen as a simple approximation of the lifted inequalities (2.13).

Proposition 2.9. *If $P \subseteq N$ is a pack for K, and α_i, $\forall\, i \in P$ are defined as in* (2.15)*, then the lifted pack inequality* (2.13) *is valid for K. Moreover, inequality* (2.13) *defines a facet of* $\operatorname{conv}(K)$ *if P is a maximal pack.*

Proof. Proof by contradiction : Assume $\exists\, \hat{\mathbf{x}} \in \left\{ X \ : \ x(N \setminus P) - \sum_{i \in P} \alpha_i(1 - x_i) < 1 \right\}$. W.L.O.G. assume the order in which the lifting coefficients were generated to be $K = \{1, 2, \ldots, |P|\}$. Now, consider $k = \max\{i \in K \ : \ \hat{x}_i = 0\}$. Now,

$$x(N \setminus P) - \sum_{i=1}^{k-1} \alpha_i(1 - x_i) < 1 + \alpha_k = \varphi(I, k) - \boldsymbol{\alpha}(\{1, 2, \ldots, k-1\})$$

$$x(N \setminus P) + \sum_{i=1}^{k-1} \alpha_i x_i < \varphi(I, k)$$

where $I = (N \setminus P) \cup \{1, 2, \dots k-1\}$. However by definition of $\varphi(I, k)$, the right hand side of the above inequality is the lower bound on the left hand side for any given feasible $\hat{\mathbf{x}} \in X$, which is the contradiction above. Hence, (2.13) is satisfied $\forall\, \mathbf{x} \in X$.

□

Corollary 2.1. *The lifted pack inequality*

$$x(N \setminus P) - \sum_{i \in P} \widehat{\alpha}_i (1 - x_i) \geq 1, \tag{2.17}$$

where $\widehat{\alpha}_k = \lceil \widehat{\varphi}(I, k) \rceil - 1 - \widehat{\boldsymbol{\alpha}}(J)$, $k \in P \setminus J$ *and* $\widehat{\varphi}(I, k)$ *is any lower bound on* $\varphi(I, k)$, *is valid for* K.

Computing the lifting coefficients α_k, $k \in P$, exactly may be computationally prohibitive in general as the feasible set of the lifting problem (2.16) is defined over a supermodular covering knapsack. For a deeper understanding of the structure of the lifted inequalities, it is of interest to identify bounds on the lifting coefficients that are independent of a chosen lifting sequence. As we shall see later, these bounds may help to generate approximate lifting coefficients quickly. We start with the following lemma.

Lemma 2.1. *Let* $P \subseteq N$ *be a maximal pack with* $\delta := d - f(P) (> 0)$ *and for* $h = 0, 1, 2, 3, \dots, |N \setminus P|$, *define*

$$\mu_h := \max \{ f(T \cup P) \; : \; |T| = h, \; T \subseteq N \setminus P \} \tag{2.18}$$

$$\nu_h := \min \{ f(T \cup P) \; : \; |T| = h, \; T \subseteq N \setminus P \}. \tag{2.19}$$

Then, for all $h = 0, 1, 2, 3, \dots, |N \setminus P| - 1$, *the following inequalities hold:*

(i) $\nu_{h+1} \geq \nu_h + \delta$,

(ii) $\mu_{h+1} \geq \mu_h + \delta$.

Proof. Since P is a maximal pack, $\rho_k(P) \geq \delta, \; \forall\, k \in N \setminus P$.

(i) Let T^*_{h+1} be an optimal solution corresponding to (2.19) and let $k \in T^*_{h+1}$. Then by supermodularity of f and maximality of P, we have

$$\begin{aligned} \delta \leq \rho_k(P) &\leq \rho_k \left((T^*_{h+1} \setminus k) \cup P \right) \\ &= f(T^*_{h+1} \cup P) - f\left((T^*_{h+1} \setminus k) \cup P \right). \end{aligned}$$

Adding ν_h to both sides yields,

$$\delta + \nu_h \leq f(T^*_{h+1} \cup P) = \nu_{h+1}.$$

(ii) Let T_h^* be an optimal solution to (2.18) and let $k \in N \setminus \{P \cup T_h^*\}$. It follows from supermodularity of f and maximality of P that

$$\begin{aligned}\delta \le \rho_k(P) &\le \rho_k(T_h^* \cup P)\\ &\le f(T_h^* \cup k \cup P) - f(T_h^* \cup P).\end{aligned}$$

Adding μ_h to both sides yields,

$$\delta + \mu_h \le f(T_h^* \cup k \cup P) \le \mu_{h+1}.$$

In summary, for a maximal pack P, $\nu_h \le f(T \cup P)$, $\forall T \subseteq N \setminus P$ with $|T| \ge h$, and $\mu_h \ge f(T \cup P)$, $\forall T \subseteq N \setminus P$ with $|T| \le h$. □

Proposition 2.10 is inspired by a similar result by Balas [15] for the linear 0-1 knapsack problem.

Proposition 2.10. *Let $P \subseteq N$ be a pack with $\delta := d - f(P) > 0$ and μ_h and ν_h, $h = 0, 1, 2, 3, \ldots, |N \setminus P|$ be defined as in* (2.18) *and* (2.19)*. Suppose that the lifted pack inequality*

$$x(N \setminus P) - \sum_{i \in P} \alpha_i (1 - x_i) \ge 1 \tag{2.20}$$

defines a facet of conv(K). For any $i \in P$, the following statements hold:

(i) if $\rho_i(\emptyset) \ge f(N) - \nu_{|N \setminus P| - h}$, then $\alpha_i \ge h$;

(ii) if $\rho_i(N \setminus i) \le \mu_{1+h} - d$, then $\alpha_i \le h$.

Proof. (i) The lifting coefficient of x_i, $i \in P$, is the smallest if x_i is the last variable introduced to (2.20) in a lifting sequence. Let $\alpha_i = \varphi(N \setminus i, i) - 1 - \boldsymbol{\alpha}(P \setminus i)$. Also, because the intermediate lifting inequality before introducing x_i is valid for K, we have $\varphi(N \setminus i, \emptyset) \ge 1 + \boldsymbol{\alpha}(P \setminus i)$. Thus, it is sufficient to show that $\varphi(N \setminus i, i) - \varphi(N \setminus i, \emptyset) \ge h$.

We claim that in any feasible solution S to the lifting problem $L(N \setminus i, i)$ (when x_i is lifted last), at least $h+1$ variables in $N \setminus P$ are positive. For contradiction, suppose that at most h variables in $N \setminus P$ are positive. Let $J \subseteq N \setminus P$ and $\tilde{P} \subseteq P \setminus i$ be such that $S = J \cup \tilde{P}$.

We have

$$\begin{aligned}
f(J \cup \tilde{P}) &\le f(J \cup P \setminus i) \\
&= f(J \cup P) - \rho_i(J \cup P \setminus i) \\
&\le f(J \cup P) - \rho_i(\emptyset) \\
&\le f(J \cup P) - f(N) + \nu_{|N \setminus P| - h} \\
&= f(P) + \rho_J(P) - f(N) + \nu_{|N \setminus P| - h} \\
&\le f(P) + \rho_J(N \setminus J) - f(N) + \nu_{|N \setminus P| - h} \\
&= f(P) - f(N \setminus J) + \nu_{|N \setminus P| - h} \\
&\le f(P) < d,
\end{aligned}$$

where the penultimate inequality follows from the fact that $f(N \setminus J) \ge \nu_{|N \setminus P| - h}$, $\forall\, J \subseteq N \setminus P$, $|J| \le h$. Thus, χ_S is infeasible for $L(N \setminus i, i)$.

Now let $S^* = J^* \cup P^*$ with $J^* \subseteq N \setminus P$, $P^* \subseteq P \setminus i$, be an optimal solution to $L(N \setminus i, i)$. Let $J \subseteq J^*$ be such that $|J| = h$. The existence of such a J is guaranteed by the argument in previous paragraph. We claim that $S^* \setminus J$ is a feasible solution to $L(N \setminus i, \emptyset)$. To see this, observe that

$$\begin{aligned}
f((S^* \setminus T) \cup i) &\ge f(S^* \setminus T) + f(i) \\
&= f(S^* \setminus T) + \rho_i(\emptyset) \\
&\ge f(S^*) - f(N) + f(N \setminus T) + \rho_i(\emptyset) \\
&\ge f(S^*) - f(N) + \nu_{|N \setminus P| - h} + \rho_i(\emptyset) \\
&\ge f(S^*) \ge d,
\end{aligned}$$

where the third inequality follows from the supermodularity of f and the penultimate inequality follows from our assumption $\rho_i(\emptyset) \ge f(N) - \nu_{|N \setminus P| - h}$. Thus, we see that $\varphi(N \setminus i, i) - \varphi(N \setminus i, \emptyset) \ge |T| = h$.

(ii) For this part, it is sufficient to show that if the pack inequality (2.4) is lifted first with x_i, then $\alpha_i \le h$. Consider the lifting problem, $L_i(N \setminus P)$. Let $T \subseteq N \setminus P$, $|T| = h + 1$, such that $f(T \cup P) = \mu_{h+1}$. We claim that T is feasible for $L_i(N \setminus P)$. Consider the following

$$\begin{aligned}
f(T \cup P \setminus i) &= f(T \cup P) - \rho_i(T \cup P \setminus i) \\
&\ge \mu_{h+1} - \rho_i(N \setminus i) \\
&\ge d.
\end{aligned}$$

Hence an optimal solution to $L_i(N \setminus P)$ has at most $h+1$ variables positive, i.e., $\varphi(N \setminus P, i) \le h + 1$. Thus we have $\alpha_i = \varphi(N \setminus P, i) - 1 \le h$. □

Computing the bounds μ_h and ν_h, $h = 1, \ldots, |N \setminus P|$ is $\mathcal{NP}$-hard as they require minimizing and maximizing supermodular functions over a cardinality restriction. Nevertheless, Lemma 2.1 and Proposition 2.10 can be utilized together in order to derive approximate lifted inequalities efficiently as μ_1, ν_1 and $\mu_{|N \setminus P|-1}$, $\nu_{|N \setminus P|-1}$ can be computed in linear time by enumeration.

Proposition 2.10 yields that for a maximal pack P if for any $i \in P$, $\rho_i(N \setminus i) \leq \mu_1 - d$, then the corresponding lifting coefficient α_i for x_i is zero and thus x_i can be dropped from consideration for extensions and lifting of the pack inequality. Similarly, if for any $i \in P$, $\rho_i(\emptyset) \geq f(N) - \nu_{|N \setminus P|-1}$, then the lifting coefficient α_i of x_i is at least one and thus x_i can be included in every extension or lifting of the pack inequality. Also, if $\rho_i(\emptyset) \geq f(N) - \nu_1$, $i \in P$, then the corresponding lifting coefficient is set to $|N \setminus P| - 1$. Furthermore, Proposition 2.10 and a repeated application of Lemma 2.1 suggest the following corollary.

Corollary 2.2. *For* $h = 1, \ldots, |N \setminus P| - 1$

1. *if* $\rho_i(\emptyset) \geq f(N) - \nu_1 - \delta(|N \setminus P| - h - 1)$, *then* $\alpha_i \geq h$.
2. *if* $\rho_i(N \setminus i) \leq \mu_1 + h\delta - d$, *then* $\alpha_i \leq h$.

2.3 Separation of Pack Inequalities

In this section, we give a separation algorithm for the pack inequalities for the supermodular covering knapsack set K defined with respect to any supermodular set function f assuming the functional form (2.2) with g concave and increasing on $\mathbb{R}_+$ and $\mathbf{c} \geq \mathbf{0}$. Observe that conic quadratic supermodular function defining K_{CQ} assumes this functional form.

Given $\bar{\mathbf{x}} \in \mathbb{R}^N$ such that $0 \leq \bar{\mathbf{x}} \leq 1$, we are interested in finding a pack P with $\sum_{i \in N \setminus P} \bar{x}_i < 1$, if there exists any. Then, the separation problem with respect to the pack inequalities can be formulated as

$$\zeta = \min \left\{ \bar{\mathbf{x}}^\top (\mathbb{1} - \mathbf{z}) \ : \ \mathbf{u}^\top \mathbf{z} - g(\mathbf{c}^\top \mathbf{z}) < d, \, z \in \{0,1\}^N \right\}, \tag{2.21}$$

where the constraint $\mathbf{u}^\top \mathbf{z} - g(\mathbf{c}^\top \mathbf{z}) < d$ ensures that a feasible $\mathbf{z}$ corresponds to a pack. Thus, there is a violated pack inequality if and only if $\zeta < 1$.

In order to find violated pack inequalities quickly, we employ a heuristic that rounds off fractional solutions to the continuous relaxation of (2.21):

$$\max \left\{ \bar{\mathbf{x}}^\top \mathbf{z} \ : \ \mathbf{u}^\top \mathbf{z} - y \leq d, \, \mathbf{c}^\top \mathbf{z} \geq h(y), \, \mathbf{0} \leq \mathbf{z} \leq \mathbf{1}, \, y \in \mathbb{R} \right\}, \tag{2.22}$$

where h is the inverse of g (h exists as g is increasing). Because g is increasing concave, h is increasing convex; hence (3.51) is a convex optimization problem. Also, observe that, for a fixed value of $y \in \mathbb{R}$, there can be at most two fractional z_i, $i \in N$ in any extreme point solution to (3.51).

For the convex relation (3.51) let $\lambda \geq 0, \nu \leq 0, \boldsymbol{\alpha} \leq \mathbf{0}, \boldsymbol{\beta} \leq \mathbf{0}$ be the dual variables for the constraints in the order listed. From the first order optimality conditions

$$\begin{aligned} \bar{x}_i - \lambda u_i - \nu c_i - \alpha_i + \beta_i = 0, \ \forall \ i \in N, \\ \lambda + \nu h'(y) = 0, \end{aligned}$$

and the complementary slackness conditions

$$\begin{aligned} \alpha_i z_i = 0, \ \forall i \in N, \\ \beta_i (z_i - 1) = 0, \ \forall i \in N, \end{aligned}$$

we see that optimal solutions satisfy

$$\bar{x}_i \begin{cases} \leq \lambda u_i + \nu c_i, & z_i = 0 \\ = \lambda u_i + \nu c_i, & 0 < z_i < 1 \\ \geq \lambda u_i + \nu c_i, & z_i = 1. \end{cases}$$

Since in an extreme point of (3.51) there are at most two variables with $0 < z_i, z_j < 1$, we compute $\binom{|N|}{2}$ candidate values for λ and ν, which are solutions of

$$\bar{x}_i = \lambda u_i + \nu c_i, \ \bar{x}_j = \lambda u_j + \nu c_j, \ i, j \in N, \, i < j.$$

For candidate values (λ, ν) satisfying $\lambda \geq 0, \ \nu \leq 0$, we assign variables $z_i, \ i \in N$ equal to one, in the non-increasing order of $\bar{x}_i / (\lambda u_i + \nu c_i)$, until $\mathbf{z}$ defines a pack and check for the violation of the corresponding pack inequality.

2.4 Computational Experiments

In this section we present our computational experiments on testing the effectiveness of the pack inequalities and their extensions for solving 0-1 optimization problems with conic quadratic covering knapsack constraints. For the computational experiments we use the MIP solver of CPLEX† (version 12.5) that solves conic quadratic relaxations at the nodes of the branch-and-bound tree. CPLEX heuristics are turned off and a single thread is used. The search strategy is set to traditional branch-and-bound, rather than the default dynamic search as it is not possible to add user cuts in CPLEX while retaining the dynamic search strategy. In addition, the solver time limit and memory limit have been set to 3600 secs. and 1 GB, respectively. All experiments are performed on a 2.93GHz Pentium Linux workstation with 8GB main memory.

In Tables 2.1 and 2.2 we report the results of the experiments for varying number of variables (n), constraints (m), and values for Ω. For each combination, five random instances are

†CPLEX is a registered trademark of IBM ILOG

generated with u_i from uniform $[0, 100]$ and σ_i from uniform $[0, u_i/5]$. The covering knapsack right-hand-side constant d is set to $0.5\,\kappa$, where $\kappa = \max_{i \in N} f(N \setminus i)$. So that constraints are not completely dense, we set the density of the constraints to $20/\sqrt{n}$.

In Table 2.1 we compare the initial relaxation gap (*igap*), the root relaxation gap (*rgap*), the end gap (*egap*), the gap between best upper bound and lower bound at termination, the number of cuts generated (*cuts*), the number of nodes explored (*nodes*), the CPU time in seconds (*time*), and the number of instances solved to optimality (#) using the barrier algorithm and several cut generation options. The initial relaxation gap (*igap*) is computed as $\frac{(f_u - f_i)}{f_u}$, where f_i denotes the objective value of the initial relaxation and f_u denotes the objective of the best feasible solution found across all versions. The root gap (*rgap*) and the end gap (*egap*) are computed as $\frac{(f_u - f_r)}{f_u}$ and $\frac{(f_u - f_l)}{f_u}$, where f_r is the objective value of the relaxation at the root node and f_l is the best lower bound for the optimal objective at termination. The columns under heading cplex show the performance of CPLEX with no user cuts added. The other columns show the performance of the algorithm using maximal pack cuts and extended maximal pack cuts with preprocessing as described in Corollary 2.2. The pack inequalities and their extensions are added only at the root node of the search tree using the separation algorithm discussed in Section 2.3.

Table 2.1: Effect of cuts with barrier algorithm.

				cplex barrier					packs						extended packs					
m	n	Ω	igap	rgap	egap	nodes	time	#	cuts	rgap	egap	nodes	time	#	cuts	rgap	egap	nodes	time	#
10	50	1	22.8	22.8	0	4,087	27	5	31	7.0	0	367	4	5	40	3.9	0	188	2	5
		3	22.4	22.4	0	4,673	29	5	28	8.6	0	338	4	5	31	5.5	0	120	2	5
		5	25.1	25.1	0	15,854	92	5	31	8.7	0	503	5	5	33	6.0	0	249	3	5
	100	1	11.4	11.4	0	153,652	2,673	2	25	7.6	0	27,394	599	5	30	6.6	0	15,214	345	5
		3	10.4	10.4	0	95,758	1,688	5	24	7.1	0	16,167	324	5	28	5.9	0	11,737	254	5
		5	11.1	11.1	0	160,024	2,726	2	22	8.1	0	50,734	1,021	5	27	7.4	0	26,763	581	5
20	50	1	18.5	18.5	0	74,833	1,209	5	51	8.2	0	4,104	98	5	59	5.8	0	2,115	55	5
		3	21.1	21.1	0.4	129,208	1,943	3	49	8.0	0	9,028	208	5	63	5.6	0	4,764	126	5
		5	21.5	21.5	0	68,563	1,043	5	48	8.1	0	1,028	26	5	55	5.2	0	433	12	5
	100	1	11.3	11.3	5.6	71,460	3,589	0	27	9.1	4	58,659	3,329	1	34	8.6	3.2	54,293	3,146	1
		3	11.3	11.3	5.2	78,661	3,589	0	35	9.1	4	66,359	3,589	0	42	8.4	3.4	61,112	3,589	0
		5	11.3	11.3	4.0	77,952	3,589	0	31	9.0	3	61,461	3,159	1	39	8.3	2.3	56,462	3,085	1
			Average	**16.5**	**1.27**	**77,894**	**1,850**			**8.2**	**0.92**	**24,679**	**1,031**			**6.4**	**0.74**	**19,454**	**933**	
			Stdev	**5.82**						**0.72**						**1.46**				

We observe in Table 2.1 that the addition of the pack cuts reduces the root gap and the number of nodes and leads to faster solution times. As expected, the extended pack cuts

Table 2.2: Effect of cuts with outer linear approximation.

				cplex outer approx.					packs						extended packs					
m	n	Ω	igap	rgap	egap	nodes	time	#	cuts	rgap	egap	nodes	time	#	cuts	rgap	egap	nodes	time	#
20	50	1	22	8.9	0	1,942	1	5	64	4.8	0	587	1	5	71	3.6	0	260	1	5
		3	24.7	10.7	0	2,792	1	5	71	6.2	0	744	1	5	82	4.3	0	396	1	5
		5	22.9	9.7	0	1,834	1	5	64	4.8	0	217	0	5	72	3.1	0	134	0	5
	100	1	11.7	7.0	0	517,570	575	5	57	6.8	0	195,698	229	5	62	6.8	0	151,307	157	5
		3	13.1	7.7	0	249,849	234	5	52	7.4	0	127,090	138	5	57	6.9	0	113,878	124	5
		5	12.4	7.0	0	242,291	211	5	50	6.7	0	106,121	126	5	61	6.4	0	94,831	105	5
30	50	1	24.2	12.4	0	3,393	3	5	67	9.7	0	1,108	1	5	84	8.4	0	572	1	5
		3	23.6	10.2	0	1,335	1	5	66	7.2	0	481	1	5	81	5.9	0	121	1	5
		5	23.9	10.8	0	2,241	2	5	67	7.3	0	368	1	5	78	6.0	0	274	1	5
	100	1	13.6	9.4	0.3	1,160,006	2,159	4	61	8.9	0.3	755,204	1,458	4	73	8.6	0.2	790,050	1,585	4
		3	12.9	8.6	0.3	1,094,672	2,238	2	67	8.2	0	686,178	1,451	4	78	8.0	0	596,803	1,195	5
		5	12.9	8.3	0	1,047,374	1,903	5	64	8.2	0	636,519	1,319	5	77	7.7	0	387,649	698	5
			Average	**9.2**	**0.05**	**360,442**	**611**			**7.2**	**0.03**	**209,193**	**394**			**6.3**	**0.02**	**178,023**	**322**	
			Stdev	**1.64**						**1.48**						**1.83**				

are more effective than the simpler pack cuts. On average, the root gap is reduced from 16.5% to 6.43% for all instances with the extended pack cuts. Using extended packs leads to a reduction of 49.5% in the solution times and 75% in the number of branch and bound nodes explored. For problems that could be solved by CPLEX alone, the average solution time is reduced from 769 seconds to mere 97 seconds. For problems that could not be solved by either of the three versions, the average end gap is reduced from 4.8% to 2.8% using the extended packs. Over all instances, the average number of nodes are $77,894$, $24,679$ and $19,454$ for CPLEX with barrier algorithm without user cuts, with packs and extended packs, respectively. On the other hand, the average CPU times are $1,850$, $1,031$ and 933 seconds for CPLEX without user cuts, with packs and extended packs, respectively.

In Table 2.2 we present similar comparisons, but this time using the CPLEX linear outer approximation for solving conic quadratic problems at the nodes instead of the barrier algorithm. We observe, in this case, that CPLEX adds its own cuts from the linear constraints. Therefore, compared to Table 2.1, in general the root gaps are smaller and the solution times are faster. Adding extended pack cuts reduces the average root gap from 9.23% to 6.31%. This leads to 50.6% reduction in the number of search nodes and 47.2% reduction in the solution times. For larger instances that are not solved to optimality, the average end gap is reduced from 0.9% to 0.3%.

In conclusion, we find the pack inequalities and their extensions to be quite effective in strengthening the convex relaxations of the conic quadratic covering 0-1 knapsacks and reducing the solution times of optimization problems with such constraints.

Chapter 3

General Submodular Knapsacks

3.1 Introduction

The submodular knapsack set is the discrete lower level set of a submodular function. Submodular and supermodular knapsack sets arise naturally when modeling utilities, risk and probabilistic constraints on discrete variables. In a recent paper Atamtürk and Narayanan [12] studied the lower level set of a non-decreasing submodular function. In Chapter 2, we explored the structure of this polyhedral set when the underlying set function is non-increasing to complement and complete the discussion on monotone submodular knapsacks. It is of interest to study the polyhedral structure of this level set when the monotonicity assumptions are relaxed. An additional application lies in form of the following second order cone set

$$S_{\text{SOC}} := \left\{\mathbf{x} \in \{0,1\}^n \ : \ \mathbf{a}^\top \mathbf{x} - \Omega\sqrt{\mathbf{x}^\top \Sigma \mathbf{x}} \geq b\right\},$$

where $\Sigma = [\sigma_{ij}]_{1\leq i,j\leq n} \succeq 0,\ a_i \geq \Omega \cdot \sigma_i \,\forall\, 1 \leq i \leq n$. This is the inner approximation of the chance constraint (1.6) when $\xi_i,\ i \in N$ are correlated.

It can be seen $S_{\text{SOC}} = S_{\text{QP}} \cap \left\{x \in \{0,1\} \ : \ \mathbf{a}^\top \mathbf{x} \geq b\right\}$, where

$$S_{\text{QP}} := \left\{\mathbf{x} \in \{0,1\}^n \ : \ \sum_i \alpha_i x_i + 2\sum_{j>i} \beta_{ij} x_i x_j \leq \gamma\right\}$$

and $\alpha_i = (2a_i b + \Omega^2\sigma_{ii}^2 - a_i^2)$, $\beta_{ij} = -(a_i a_j - \Omega^2 \sigma_{ij}) \leq (\Omega^2 \sigma_i \sigma_j - a_i a_j) \leq 0$ and $\gamma = b^2$.

Proposition 3.1. (Fisher, Nemhauser and Wolsey, 1978 [72])
Consider a set function $f : \{0,1\}^n \mapsto \mathbb{R}$, defined as a binary quadratic mapping,

$$f(\mathbf{x}) := \mathbf{x}^\top Q\, x \tag{3.1}$$

where Q is a $n \times n$ off-diagonal matrix. $f(\cdot)$ is submodular if and only if

$$Q_{ij} \leq 0,\ 1 \leq i,\ j\ \leq n.$$

Proof. Consider, $S \subseteq T \subseteq N \setminus i \quad$ for some $i \in N$.

$$\begin{aligned}\rho_i(T) - \rho_i(S) &= f(T \cup i) - f(S \cup i) - f(T) + f(S)\\ &= Q_{i(j \in T)} - Q_{i(j \in S)}\\ &= Q_{i(j \in T \setminus S)}\\ &\leq 0\end{aligned}$$

where the last inequality follows from non-positivity of $Q_{ij} \leq 0,\ 1 \leq i, j \leq n$. Thus, we have $\rho_i(S) \leq \rho_i(T) \ \ \forall\ S \subseteq T \subseteq N \setminus i \quad i \in N$ proving submodularity of $f(\cdot)$.

Alternatively, assume $f(\cdot)$ is submodular, thus $\forall\ S \subseteq T \subseteq N \setminus i \quad i \in N$

$$\begin{aligned}0 &\leq \rho_i(S) - \rho_i(T)\\ 0 &\leq f(S \cup i) - f(T \cup i) - f(S) + f(T)\\ 0 &\leq Q_{i(j \in S)} - Q_{i(j \in T)}\\ 0 &\geq Q_{i(j \in T \setminus S)}\end{aligned}$$

Thus, $Q_{i(j \in T \setminus S)} \leq 0$, $\forall\ S \subseteq T \subseteq N \setminus i \quad i \in N$, which yields $Q_{ij} \leq 0,\ 1 \leq i, j \leq n$. $\square$

Corollary 3.1. *Consider a set function $f : \{0,1\}^n \mapsto \mathbb{R}$, defined as a binary quadratic mapping*

$$f(\mathbf{x}) := \mathbf{a}^\top x + \mathbf{x}^\top Q\, x, \tag{3.2}$$

where Q is a $n \times n$ matrix and $\mathbf{a} \in \mathbb{R}$. $f(\cdot)$ is submodular if and only if

$$Q_{ij} \leq 0,\ 1 \leq i, j \leq n\,,\, i \neq j.$$

Proposition 3.1 and Corollary 3.1 in effect suggest that S_{QP} is the lower level set of a submodular set function. The associated set however is not necessarily monotone. A requirement to study the polyhedral structure of the level sets associated with the generic submodular set functions is thus apparent. Albeit the motivation stems from the submodular quadratic maps, the following discussion is valid for knapsack sets associated with submodular functions in general.

3.2 Linear 0-1 Knapsack Set

The knapsack problem is one of the most celebrated problems in optimization literature. Most of the literature available on the knapsack problem is for the linear knapsack set (binary, integer, mixed-integer). The polyhedral analysis of the linear knapsack set was initiated by Balas [15, 17], Hammer et al. [45], and Wolsey [95]. For an extensive review of theoretical and computational results on linear knapsacks we refer the reader to [6, 5, 42, 65]. In this section we'll review the results and literature for the case of linear $0-1$ knapsack set $K := \left\{\mathbf{x} \in \{0,1\}^n \ : \ \mathbf{a}^\top \mathbf{x} \leq b\right\}, \mathbf{a} \geq 0$.

In the following, we review some of the results on the valid inequalities for $\text{conv}(K)$

Proposition 3.2. *Inequality $x_i \geq 0$, $i \in N$ is facet defining for* $\text{conv}(K)$.

Proposition 3.3. *Inequality $x_i \leq 1$, $i \in N$ is facet defining for* $\text{conv}(K)$ *if and only if $a_i + a_j \leq b$, $\forall\ j \in N \setminus \{i\}$.*

Proposition 3.4. *If the inequality $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a facet for* $\text{conv}(K)$ *not including* $\mathbf{0}$ *then $\beta > 0$ and $\alpha_j \geq 0$, $\forall\ j \in N$.*

3.2.1 Cover Inequalities

Definition 3.1. A subset C of the index set N is called a *cover* if $\lambda := a(C) - b > 0$.

For a cover C, let us consider the restriction K_C obtained by fixing all x_i, $i \in N \setminus C$ to zero. Since the sum of the coefficients a_i, $i \in C$ exceeds the knapsack capacity by $\lambda > 0$, all variables x_i, $i \in C$ cannot take a value of one simultaneously for any $\mathbf{x} \in K$. Therefore, the *cover inequality* [15, 45, 95]

$$x(C) \leq |C| - 1 \tag{3.3}$$

is valid for $\text{conv}(K)$. Cover inequality defines a facet for $\text{conv}(K_C)$ if and only if C is a minimal cover, that is, $\mathbf{a}(C \setminus \{i\}) \leq b$, $\forall\, i \in C$.

Extensions of Cover Inequalities

Extensions are a means to strengthen the inequalities based on restrictions of feasible sets, in this case the cover inequalities. For a cover $C \subseteq N$, consider the cover inequality (3.3).

$$\mathbf{x}(C) \leq |C| - 1$$

An important and very useful concept in deriving strong valid inequalities is lifting of inequalities. Lifting refers to extending valid inequalities for low dimensional restrictions of polyhedra to ones that are valid in high dimensions. The concept of lifting has been introduced by Gomory [40] in the context of the group problem. Padberg [74] described the sequential lifting procedure for $0-1$ programming. Since then lifting has been studied and used extensively (Atamtürk [7]; Balas and Zemel, [17]; Escudero, Garín, and Péres, [38]; Gu, Nemhauser, and Savelsbergh,[43, 41, 42, 44]; Johnson and Padberg, [51]; Louveaux and Wolsey, [62]; Marchand and Wolsey, [64]; Nemhauser and Vance, [69]; Padberg, [75]; Richard, de Farias, and Nemhauser, [77]; Sherali and Lee, [83]; Wolsey, [95, 98]; Zemel, [101, 100]), particularly, for $0-1$ and mixed $0-1$ programming problems. We can strengthen the cover inequality by introducing the variables not present in the inequality (x_i, $\forall\, i \in N \setminus C$) multiplied with appropriate coefficients. The lifted cover inequality in this case can be represented as

$$\mathbf{x}(C) + \sum_{i \in N \setminus C} \alpha_i x_i \leq |C| - 1, \tag{3.4}$$

where $\alpha_i \geq 0$, $i \in N \setminus C$ are the corresponding lifting coefficients. Obtaining exact lifting coefficients entails computing the lifting function $\Theta(\cdot)$ of cover inequality (3.3)

$$\Theta(a) \ := \ |C| - 1 - \max\left\{\sum_{i \in C} x_i \ : \ \sum_{i \in C} a_i x_i \leq b - a\right\} \tag{3.5}$$

for $a \geq 0$. Obtaining a closed form expression for the lifting function is not always trivial. Extensions are computationally inexpensive special cases of lifting, wherein instead of deriving the exact lifting coefficients, we identify whether a variable x_i, $i \in N \setminus C$ can be introduced into the cover inequality with a coefficient $\alpha_i \geq 1$. Let E be a set of all such indices, i.e. $E := \{i \in N \setminus C \ : \ \alpha_i \geq 1\}$. The extended cover inequality thus is

$$\mathbf{x}(C \cup E) \leq |C| - 1. \tag{3.6}$$

Consider a subset of indices $\overline{E} \subseteq N \setminus C$. Assume that the corresponding variables x_i, $i \in \overline{E}$ have been included in the extended cover inequality. Consider the variable x_k, $k \in N \setminus (C \cup \overline{E})$ to be included next in the extended cover.

Proposition 3.5. $\alpha_k \geq 1$, *if* $a_k > \max_{j \in C \cup \overline{E}} a_j - \lambda$

Atamtürk [5], Balas and Zemmel [17], Gu et al. [44] provide a characterization of the lifting function $\Theta(a)$ for the cover inequalities for $0-1$ integer knapsack set. This characterization yields a sequence independent lifting procedure, and as a special case, a sequence independent extension for the cover inequalities. Attributed to this, we can further simplify the extension procedure to a sequence independent extension.

Corollary 3.2. *For* $k \in N \setminus C$, $\alpha_k \geq 1$, *if* $a_k \geq \max_{j \in C} a_j$.

The corresponding extension set $E \subseteq N \setminus C$ can now be defined as

$$E \ := \left\{i \ \in \ N \setminus C \ : \ a_i \geq \max_{j \in C} a_j\right\}. \tag{3.7}$$

Proposition 3.6. *The extended cover inequality* (3.6) *is valid for* $\mathrm{conv}(K)$. *In addition, inequality* (3.6) *defines a facet of* $\mathrm{conv}(K_{C \cup E})$ *if and only if* C *is minimal and* $\forall\, i \in E$ $\exists$ *distinct* $\{j, k\} \in C$ *such that* $\mathbf{a}(C \cup \{i\} \setminus \{j, k\}) \leq b$.

Sequence Independent Bounds for Lifting Coefficients

As a follow up to extensions, it is of interest to understand whether the lifting coefficients α_i, $i \in N \setminus C$ in the lifted cover inequality (3.4) can be computed efficiently in general. Sequential lifting and simultaneous lifting of cover inequalities have been studied extensively (Balas, [15]; Balas and Zemel, [17, 18]; Gu, Nemhauser, and Savelsbergh, [43, 42]; Hammer, Johnson, and Peled, [45]; Wolsey, [95]; Zemel, [100]) to extend them to strong inequalities for conv(K). Wolsey [98] introduced the idea of superadditivity to strengthen valid inequalities for $0-1$ integer programs. Gu et al. [44] and Atamtürk [7] have explored the idea of superadditive lifting further in relation to mixed integer programming.

Atamtürk [5] present a unified review of the inequalities, whilst focusing on the use of superadditive functions for the analysis of knapsack polyhedra. They present a superadditive lower bound on the lifting function for cover inequalities. Following is a direct consequence of the subadditive lower bound $\varphi(\cdot)$ on the lifting function $\Theta(\cdot)$ which can be used to obtain lower bounds on the lifting coefficients α_i, $i \in N \setminus C$.

Proposition 3.7. *For $k \in N \setminus C$, $\alpha_k \geq h$, if $a_k \geq A_h$, where $A_h = \max\limits_{\substack{T \subseteq C \\ |T|=h}} \mathbf{a}(T)$.*

Observe that A_h, $0 \leq h \leq |N|$ can be efficiently computed using greedy algorithm since $a_i \geq 0,\ i \in N$. Conversely, to obtain an upper bound on the lifting coefficients, consider the lifting function $\Theta(a)$ (3.5). It is easy to observe that any feasible solution to the optimization problem

$$\max \left\{ \sum_{i \in C} x_i \ : \ \sum_{i \in C} a_i x_i \leq b - a \right\} \tag{3.8}$$

provides an upper bound on $\Theta(a)$. A greedy algorithm yields a feasible solution to (3.8). Consider $T \subseteq S$ such that $|T| = h$. It can be seen that $\alpha_k \leq |C| - 1 - h$, if $\mathbf{a}(T) \leq b - a_k$ for $k \in N \setminus C$ for all possible lifting sequences. This yields the following result.

Proposition 3.8. *For $k \in N \setminus C$, $\alpha_k \leq h$, if $a_k \leq b - B_{|C|-1-h}$, where $B_h = \min\limits_{\substack{T \subseteq C \\ |T|=h}} \mathbf{a}(T)$.*

As earlier, B_h can be computed efficiently using a greedy approach.

The motivation for deriving these bounds will become more apparent in Section 3.3.8 where we will derive sequence independent lifting coefficients for submodular knapsack polytope, since deriving exact lifting coefficients for the submodular knapsack polytope can be computationally intractable.

3.2.2 Pack Inequalities

As seen in previous section, covers in effect are infeasible sets, and cover inequalities (3.3) are valid inequalities obtained from these infeasible sets. Contrary to that, we can also derive valid inequalities related to the feasible sets termed as *packs*. These inequalities have been studied in different forms and by different names in the literature *viz.* weight inequalities [94], reverse-cover inequalities [64], pack inequalities [5]. We refer to these feasible sets as packs through out the following discussion, starting with the preliminaries.

Definition 3.2. A subset P of the index set N is called a *pack* if $\delta := b - \mathbf{a}(P) > 0$.

For a pack P, consider the restriction K_P, obtained by fixing all x_i, $i \in P$ to one. Since any x_i, $i \in N \setminus P$ with coefficient a_i greater than the residual capacity δ cannot take the value one in a feasible solution to K_P, the *weight inequality* [94]/*pack inequality* [5]

$$\sum_{i \in N \setminus P} (a_i - \delta)^+ x_i \leq 0 \tag{3.9}$$

is valid for $\mathrm{conv}(K_P)$. Weismantel [94] extended these inequalities to derive valid inequalities for $\mathrm{conv}(K)$, their main result on reduction of weight inequalities,

Proposition 3.9. [Weismantel [94]] *Let $P \subseteq N$ satisfy $\mathbf{a}(P) < b$ and the index set $M := \{i \in N \setminus P \ : \ a_i > \delta\} \neq \emptyset$ where $\delta = b - \mathbf{a}(P)$. For an item $k \in P$ such that $a_k \geq a_i$ for all $i \in P$ and $\psi \in [0, \delta]$ with $a_k - \psi > 0$ the weight-reduction inequality with respect to T (and k) and ψ is defined as*

$$\sum_{i \in P \setminus \{k\}} a_i x_i + (a_k - \psi) x_k + \sum_{j \in M} c_j x_j \leq \mathbf{a}(P) - \psi, \tag{3.10}$$

where

$$c_j = \begin{cases} (a_j - \delta), & \text{if } \delta < a_j \leq a_k + \delta - \psi, \\ (a_j - \psi), & \text{if } a_k + \delta - \psi < a_j \leq a_k + \delta, \\ (a_j - \delta - \psi), & \text{if } a_j > a_k + \delta. \end{cases}$$

The weight reduction inequality with respect to T and ψ is valid for $\mathrm{conv}(K)$.

Atamtürk [5] strengthened the result of Weismantel [94] *via* superadditive lifting of the inequality (3.9).

Proposition 3.10 (Atamtürk [5]). *Suppose $\{i \in N \setminus P \ : \ a_i > \delta\} = \{1, 2, \ldots, q\}$ and $a_1 \geq a_2 \geq \ldots \geq a_q$. Then let $A_i = -\sum_{k=1}^{i} a_k$ for $i \in \{1, 2, \ldots, q\}$ and $A_0 = 0$. The inequality*

$$\sum_{i \in P} \psi(-a_i)(1 - x_i) + \sum_{i \in N \setminus P} (a_i - \delta)^+ x_i \leq 0$$

is valid for conv(K) *where,*

$$\psi(a) = \begin{cases} i\delta + a, & \text{if } A_{i+1} + \delta \leq a \leq A_i, \\ i\delta + A_i, & \text{if } A_i \leq a \leq A_i + \delta, \\ q\delta + A_q, & \text{if } a \leq A_q + \delta. \end{cases}$$

is the superadditive lower bound on the lifting function of weight inequality (3.9).

In the following, we will discuss the inequalities obtained from aforementioned feasible sets, and derive extensions and sequence independent bounds on lifting coefficients as in the case of covers. To begin with, consider the index set $M := \{i \in N \setminus P \ : \ a_i > \delta\}$

$$\sum_{i \in M} x_i \leq 0 \tag{3.11}$$

is an alternate version of the weight inequality (3.9) and is thus valid for K_P. We term the class of inequalities (3.11) derived from feasible sets (packs) as *pack inequalities*. Furthermore, pack inequality defines a facet of K_P if and only if P is a maximal pack, that is, $\mathbf{a}(P \cup \{i\}) > b$, $\forall\, i \in N \setminus P$.

Extensions of Pack Inequalities

Pack inequalities obtained from the feasible lower dimensional restrictions of the knapsack set K are valid for the respective restrictions. Lifting of pack inequalities is thus necessary to obtain valid inequalities for *conv*(K). Atamtürk [5] explore superadditive lower bounds for the lifting functions of the weight inequality (3.9) to derive the valid inequalities for conv(K).

For a pack $P \subseteq N$ and the index set M as defined in Section 3.2.2, consider the pack inequality (3.11).

$$\mathbf{x}(M) \leq 0$$

As in the case of cover inequalities, we can strengthen the above inequality by introducing the variables not present in the inequality (x_i, $\forall\, i \in N \setminus M$) multiplied with appropriate coefficients. A trivial procedure to extend the pack inequality (3.11) is by extending the pack P to obtain a maximal pack $\overline{P}$ (if $\exists\ a_j \leq \delta,\ j \in N \setminus P$ define $\overline{P} = P \cup \{j\}$) and $\bar{\delta} = b - \mathbf{a}(\overline{P})$. The corresponding *maximal pack inequality*

$$\mathbf{x}(N \setminus \overline{P}) \leq 0. \tag{3.12}$$

The maximal pack inequality can further be lifted to the lifted pack inequality

$$\mathbf{x}(N \setminus \overline{P}) - \sum_{i \in \overline{P}} \alpha_i (1 - x_i) \leq 0,$$

where α_i, $i \in \overline{P}$ are the corresponding lifting coefficients. The lifting function of (3.12) can be expressed as

$$\Lambda(a) = \max\left\{ \mathbf{x}(N \setminus \overline{P}) \;:\; \sum_{i \in N \setminus \overline{P}} a_i x_i \leq \bar{\delta} + a \right\} \tag{3.13}$$

for $a \geq 0$.

Define

(i) $\overline{A}_i = \min\left\{ \mathbf{a}(T) \;:\; T \subseteq N \setminus \overline{P},\, |T| = i \right\}$

(ii) $\overline{B}_i = \max\left\{ \mathbf{a}(T) \;:\; T \subseteq N \setminus \overline{P},\, |T| = i \right\}$

Observe that $\overline{A}_i$ and $\overline{B}_i$ can both be computed efficiently by a greedy approach. Suppose (without loss of generality) $N \setminus \overline{P} = \{1, 2, 3, \ldots, m\}$ and $a_1 \geq a_2 \geq \ldots \geq a_m$. Then $\overline{A}_i = \sum_{j=m-i+1}^{m} a_j$ and $\overline{B}_i = \sum_{j=1}^{i} a_i$ with $\overline{A}_0 = \overline{B}_0 = 0$. The lifting function $\Lambda(a)$, $a \geq 0$, can be expressed in closed form as

$$\Lambda(a) = \begin{cases} 0, & \text{if } \overline{A}_0 \leq a < \overline{A}_1 - \bar{\delta}, \\ i, & \text{if } \overline{A}_i - \bar{\delta} \leq a < \overline{A}_{i+1} - \bar{\delta}, \\ m, & \text{if } \overline{A}_m - \bar{\delta} \leq a. \end{cases} \tag{3.14}$$

$\Lambda(\cdot)$ is a step function, however $\psi(\cdot)$ defined as

$$\psi(a) = \begin{cases} i + \left(\frac{a - \overline{A}_i}{\overline{A}_{i+1} - \overline{A}_i - \bar{\delta}} \right), & \text{if } \overline{A}_i \leq a \leq \overline{A}_{i+1} - \bar{\delta}, \\ i, & \text{if } \overline{A}_i - \bar{\delta} \leq a \leq \overline{A}_i, \\ m, & \text{if } \overline{A}_m - \bar{\delta} \leq a. \end{cases} \tag{3.15}$$

for $a \geq 0$, and $i \in \{0, 1, 2 \ldots, m-1\}$ represents a subadditive upper bound on $\Lambda(a)$.

Proposition 3.11. *The lifted pack inequality*

$$\mathbf{x}(N \setminus \overline{P}) - \sum_{i \in \overline{P}} \psi(a_i)(1 - x_i) \leq 0 \tag{3.16}$$

is valid for $\operatorname{conv}(K)$*. In addition,* (3.16) *defines a* $n - m - 1$ *dimensional face of* $\operatorname{conv} K$ *if* $A_{i_k} - \bar{\delta} \leq a_k \leq A_{i_k}$*, for some* $i_k \in \{0, 1, 2, \ldots, m-1\}$ *for all* $k \in \overline{P}$*.*

As in the case of cover inequalities, a computationally inexpensive procedure to lift maximal pack inequalities is to identify whether a variable x_i, $i \in \overline{P}$ can be introduced into

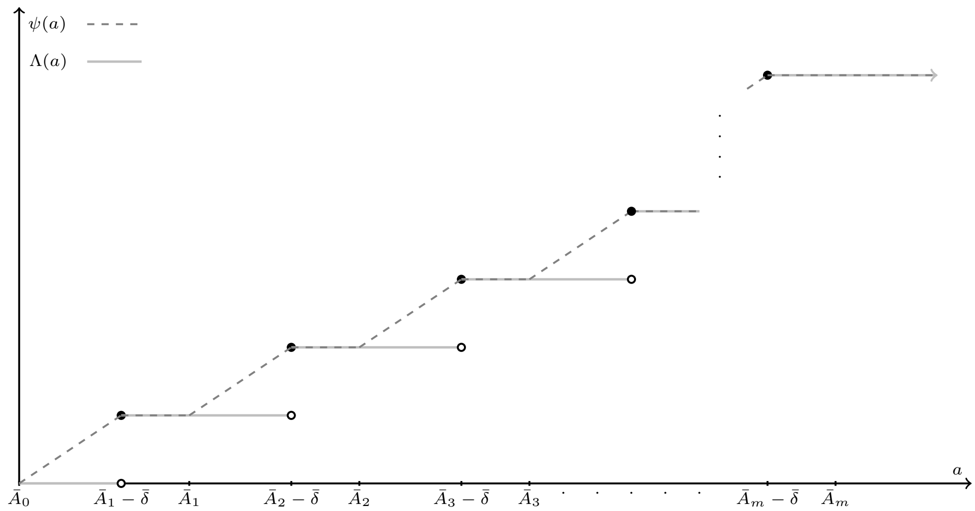


Figure 3.1: Lifting function $\Lambda(a)$ and subadditive upper bound $\psi(a)$, $a \geq 0$

the maximal pack inequality with a coefficient $\alpha_i \geq 1$. Let E be a set of all such indices, i.e. $E := \{i \in \overline{P} \ : \ \alpha_i \geq 1\}$. The extended pack inequality thus is

$$\mathbf{x}(E \cup (N \setminus \overline{P})) \leq |E|. \tag{3.17}$$

Consider a subset of indices $\overline{E} \subseteq \overline{P}$. Assume that the corresponding variables x_i, $i \in \overline{E}$ have been included in the extended cover inequality. Consider the variable $x_k, k \in \overline{P} \setminus \overline{E})$ to be included next in the extended cover.

Proposition 3.12. $\alpha_k \geq 1$, *if* $a_k + \bar{\delta} \geq \max\limits_{j \in N \setminus \overline{P}} a_j$.

where $\bar{\delta} := b - a(\overline{P})$ is the residual capacity of the maximal pack. The corresponding extension set $E \subseteq \overline{P}$ can now be defined as

$$E := \left\{ i \in \overline{P} \ : \ a_i + \bar{\delta} \geq \max_{j \in N \setminus \overline{P}} a_j \right\}. \tag{3.18}$$

Proposition 3.13. *The extended pack inequality* (3.17) *is valid for* $\mathrm{conv}(K_{\overline{P} \setminus E})$. *In addition, inequality* (3.17) *defines a facet of* $\mathrm{conv}(K_{\overline{P} \setminus E})$ *if and only if* $\overline{P}$ *is maximal and* $\forall\, i \in E$ $\exists$ *distinct* $\{j, k\} \in N \setminus \overline{P}$ *such that* $\mathbf{a}(\overline{P} \cup \{j, k\} \setminus \{i\}) > b$.

Sequence Independent Bounds on the Lifting Coefficients

As in the case of covers, it is of interest to determine sequence independent bounds on the lifting coefficients of the lifted pack inequality (3.13). The particular bounds can be obtained using the lifting function $\Lambda(\cdot)$ and the subadditive upper bound $\psi(\cdot)$. Observe that any feasible solution to max $\left\{\mathbf{x}(N \setminus \overline{P}) \;:\; \sum_{i \in N \setminus \overline{P}} a_i x_i \leq \bar{\delta} + a_j\right\}$ provides a lower bound on the lifting coefficient α_j, $j \in \overline{P}$. Alternatively, the subadditive upper bound $\psi(a_j)$ yields an upper bound on α_j, $j \in \overline{P}$. Consider the following

Proposition 3.14. *Suppose that $\overline{P} \subseteq N$ is a maximal pack, and the lifted pack inequality* (3.13) *defines a $n - m - 1$ dimensional face of* $\text{conv}(K)$*, then the following statements hold for all α_j, $j \in \overline{P}$*

(i) $\alpha_j \leq h$*, if* $a_j \leq \overline{A}_h$.

(ii) $\alpha_j \geq h$*, if* $a_j \geq \overline{B}_h - \bar{\delta}$.

Proof. (i) Follows from the definition of subadditive upper bound $\psi(a_j)$, $j \in \overline{P}$.
(ii) Consider $T \subseteq S$ such that $|T| = h$. Observe that, for $j \in \overline{P}$, $\alpha_j \geq h$, if $a(T) \leq \bar{\delta} + a_j$ for all possible lifting sequences. In other words

$$\alpha_j \geq h \quad \text{if } \max_{\substack{T \subseteq N \setminus \overline{P} \\ |T| = h}} \mathbf{a}(T) \leq a_j + \bar{\delta}$$

$$\alpha_j \geq h \quad \text{if } \overline{B}_h \leq a_j + \bar{\delta}.$$

The result follows. □

Corollary 3.3. *The extended pack inequality,*

$$\mathbf{x}(N \setminus \overline{P}) + \sum_{j \in \overline{P}} c_j x_j \leq \mathbf{c}(\overline{P}) \tag{3.19}$$

is valid for $\text{conv}(K)$*, where* $c_j = h$*, if* $\overline{A}_h \leq a_j \leq \overline{B}_h - \bar{\delta},\ j \in \overline{P}$.

3.2.3 Generalizing the Linear 0-1 Knapsack

In this section, we present a more general expression for the cover inequalities whilst relaxing the earlier assumption of $\mathbf{a} > 0$. While this is a trivial exercise for the reader, and these expressions can be readily obtained via complementing variables x_i where corresponding $a_i < 0$, we present the following results to provide a sense of completeness to this analysis.

Reconsider the knapsack set K, with $\mathbf{a} \in \mathbb{R}$.

Define the indexed sets, I^+ and I^- as following

$$I^+ := \{i \in N \;:\; a_i > 0\} \quad I^- = N \setminus I^+ := \{i \in N \;:\; a_i < 0\}.$$

The knapsack set K can be redefined for the aforementioned indexed sets as following

$$K = \left\{ \mathbf{x} \in \{0,1\}^n \ : \ \sum_{i \in I^+} a_i x_i + \sum_{j \in I^-} |a_j| \bar{x}_j \leq b + \sum_{j \in I^-} |a_j| \right\}, \tag{3.20}$$

where $\bar{x}_j = 1 - x_j$, $\forall\, j \in I^-$.

Proposition 3.15. *Inequality $x_i \geq 0$, $i \in I^+$ is facet defining for* $\text{conv}(K)$.

Proposition 3.16. *Inequality $x_i \leq 1$, $i \in I^-$ is facet defining for* $\text{conv}(K)$.

Proposition 3.17. *Inequality $x_i \leq 1$, $i \in I^+$ is facet defining for* $\text{conv}(K)$ *if and only if* $a_i + |a_k| \leq b + |\mathbf{a}|(I^-)$, $\forall\, k \in N \setminus \{i\}$.

Proposition 3.18. *Inequality $x_i \geq 0$, $i \in I^-$ is facet defining for* $\text{conv}(K)$ *if and only if* $|a_i| + |a_k| \leq b + |\mathbf{a}|(I^-)$, $\forall\, k \in N \setminus \{i\}$.

Proposition 3.19. *If the inequality $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a facet for* $\text{conv}(K)$ *not including* $\mathbf{0}$ *then $\beta > \boldsymbol{\alpha}(I^-)$, $\alpha_i \geq 0$, $\forall\, i \in I^+$ and $\alpha_j \leq 0$, $\forall\, j \in I^-$.*

Cover Inequalities, $\mathbf{a} \in \mathbb{R}$

Consider sets, $C^+ \subseteq I^+$ and $C^- \subseteq I^-$, such that $C^+ \cup C^-$ constitutes a cover, i.e.

$$\begin{aligned}
\sum_{i \in C^+} a_i + \sum_{j \in C^-} |a_j| \qquad & > b + \sum_{j \in I^-} |a_j| \\
\sum_{i \in C^+} a_i - \sum_{j \in I^- \setminus C^-} |a_j| \quad & > b \\
\sum_{i \in C^+} a_i + \sum_{j \in I^- \setminus C^-} a_j \quad & > b \\
\sum_{i \in C^+ \cup I^- \setminus C^-} a_i \quad & > b.
\end{aligned}$$

then, the corresponding cover inequality can be expressed as

$$\begin{aligned}
\sum_{i \in C^+} x_i + \sum_{j \in C^-} \bar{x}_j &\leq |C^+ \cup C^-| - 1 \\
\sum_{i \in C^+} x_i + \sum_{j \in C^-} (1 - x_j) &\leq |C^+| + |C^-| - 1 \\
\sum_{i \in C^+} x_i - \sum_{j \in C^-} x_j + |C^-| &\leq |C^+| + |C^-| - 1 \\
\sum_{i \in C^+} x_i - \sum_{j \in C^-} x_j &\leq |C^+| - 1.
\end{aligned}$$

The following result follows

Proposition 3.20. *The* generalized cover inequality

$$\mathbf{x}(C^+) - \mathbf{x}(C^-) \leq |C^+| - 1. \tag{3.21}$$

is valid for conv(K). *Furthermore, inequality* (3.21) *defines a facet for* conv $K_{C^+ \cup C^-}$ *if and only if* $C^+ \cup C^-$ *is of minimal cardinality, i.e.*

$$|a_i| \geq \lambda, \quad \forall\, i \in C^+ \cup C^-, \text{ where } \lambda = \mathbf{a}(C^+ \cup (I^- \setminus C^-)) - b.$$

It can also be seen that the corresponding the generalized lifted cover inequality in this case can be represented as

$$\mathbf{x}(C^+) + \sum_{i \in I^+ \setminus C^+} \alpha_i x_i + \sum_{j \in I^- \setminus C^-} \alpha_j \bar{x}_j - \mathbf{x}(C^-) \leq |C^+| - 1$$
$$\mathbf{x}(C^+) + \sum_{i \in I^+ \setminus C^+} \alpha_i x_i + \sum_{j \in I^- \setminus C^-} \alpha_j (1 - x_j) - \mathbf{x}(C^-) \leq |C^+| - 1$$
$$\mathbf{x}(C^+) + \sum_{i \in I^+ \setminus C^+} \alpha_i x_i - \sum_{j \in I^- \setminus C^-} \alpha_j x_j - \mathbf{x}(C^-) \leq |C^+| - \boldsymbol{\alpha}(I^- \setminus C^-) - 1$$

which yields the generalized lifted cover inequality

$$\mathbf{x}(C^+) + \sum_{i \in I^+ \setminus C^+} \alpha_i x_i - \sum_{j \in I^- \setminus C^-} \alpha_j x_j - \mathbf{x}(C^-) \leq |C^+| - (\boldsymbol{\alpha}(I^- \setminus C^-) + 1), \tag{3.22}$$

where $\alpha_i \geq 0$, $i \in I^+ \setminus C^+$ and $\alpha_j \geq 0$, $j \in I^- \setminus C^-$ are the corresponding lifting coefficients. Let E be a set of all such indices, i.e. $E := \{i \in N \setminus (C^+ \cup C^-) \ : \ \alpha_i \geq 1\}$.

Sequence independent extensions for this generalization can also be obtained in a manner similar to Section 3.2.1. We characterize the extension set E with respect to $(C^+ \cup C^-)$ as

$$E := \left\{ i \in N \setminus (C^+ \cup C^-) \ : \ |a_i| \geq \max_{j \in C^+ \cup C^-} |a_j| \right\}. \tag{3.23}$$

Further define subsets E^+ and E^- as

$$E^+ := I^+ \cap E \quad E^- := I^- \cap E.$$

The *generalized extended cover inequality* can now be expressed as

$$\mathbf{x}(C^+ \cup E^+) + \bar{\mathbf{x}}(C^- \cup E^-) \leq |C^+| + |C^-| - 1$$
$$\mathbf{x}(C^+ \cup E^+) + |C^- \cup E^-| - \mathbf{x}(C^- \cup E^-) \leq |C^+| + |C^-| - 1$$
$$\mathbf{x}(C^+ \cup E^+) + |C^-| + |E^-| - \mathbf{x}(C^- \cup E^-) \leq |C^+| + |C^-| - 1$$
$$\mathbf{x}(C^+ \cup E^+) - \mathbf{x}(C^- \cup E^-) \leq |C^+| - (|E^-| + 1).$$

The following result is immediate.

Proposition 3.21. *The generalized extended cover inequality*

$$\mathbf{x}(C^+ \cup E^+) - \mathbf{x}(C^- \cup E^-) \leq |C^+| - (|E^-| + 1) \tag{3.24}$$

is valid for $\text{conv}(K)$. *In addition, inequality* (3.24) *defines a facet of* $\text{conv}(K_{C^+ \cup C^- \cup E^+ \cup E^-})$ *if and only if* $C^+ \cup C^-$ *is of minimal cardinality and* $\forall\, i \in E^+ \cup E^-$ $\exists$ *distinct* $\{j, k\} \in C^+ \cup C^-$ *such that* $|\mathbf{a}|(C^+ \cup C^- \cup \{i\} \setminus \{j, k\}) \leq b + |\mathbf{a}|(I^-)$.

Sequence Independent Bounds on Lifting Coefficients

As a direct generalization of the results presented in Section 3.2.1 we present the following conditions to provide sequence independent bounds on the lifting coefficients of the lifted cover inequality (3.22)

$$\mathbf{x}(C^+) + \sum_{i \in I^+ \setminus C^+} \alpha_i x_i - \sum_{j \in I^- \setminus C^-} \alpha_j x_j - \mathbf{x}(C^-) \leq |C^+| - (\boldsymbol{\alpha}(I^- \setminus C^-) + 1),$$

where $\alpha_i \geq 0$, $i \in I^+ \setminus C^+$ and $\alpha_j \geq 0$, $j \in I^- \setminus C^-$ are the corresponding lifting coefficients.

To obtain the lower bounds on the aforementioned lifted coefficients, we use the alternate representation of the linear $0-1$ knapsack (3.20). Proposition 3.7 and Proposition 3.8 can be readily extended to this case to yield lower and upper bounds on the lifting coefficients, α_i, $i \in N \setminus (C^+ \cup C^-)$.

Definition 3.3. Let $(C^+ \cup C^-) \subseteq N$ be of minimal cardinality such that

$$\mathbf{a}(C^+ \cup (I^- \setminus C^-)) > b.$$

For $h = 0, 1, 2, 3, \ldots, |(C^+ \cup C^-)|$, define

$$A_h := \max\{|\mathbf{a}|(T) \,:\, T \in \mathcal{T}_h\}, \tag{3.25}$$

$$B_h := \min\{|\mathbf{a}|(T) \,:\, T \in \mathcal{T}_h\}, \tag{3.26}$$

where $\mathcal{T}_h := \{T \,:\, |T| = h,\ T \subseteq (C^+ \cup C^-)\}$.

Proposition 3.22. *Let* $(C^+ \cup C^-) \subseteq N$ *be a cover with* $\lambda := \mathbf{a}(C^+ \cup (I^- \setminus C^-)) - b$ *and* A_h *and* B_h, $h = 0, 1, 2, 3, \ldots, |C^+ \cup C^-|$ *be defined as in* (3.25) *and* (3.26). *Suppose that the lifted pack inequality* (3.22) *defines a facet of* $\text{conv}(K)$. *Then, for* $k \in N \setminus (C^+ \cup C^-)$, *the following statements hold:*

(i) If $|a_k| \geq A_h$, *then* $\alpha_k \geq h$.

(ii) If $|a_k| \leq b + |\mathbf{a}|(I^-) - B_{|C^+ \cup C^-| - 1 - h}$, *then* $\alpha_k \leq h$.

Pack Inequalities, $\mathbf{a} \in \mathbb{R}$

Akin to the cover inequalities presented for K, $\mathbf{a} \in \mathbb{R}$ above, we can rewrite the pack inequalities similarly, i.e. *(via. complementation)*

Reconsider the knapsack set K, with $\mathbf{a} \in \mathbb{R}$. Apropos of the index sets I^+ and I^- and corresponding feasible set K (3.20) defined earlier in Section 3.2.3

Consider now, $P^+ \subseteq I^+$ and $P^- \subseteq I^-$, such that $P^+ \cup P^-$ defines a pack, i.e.

$$\begin{aligned}
\sum_{i \in P^+} a_i + \sum_{j \in P^-} |a_j| \quad &< b + \sum_{j \in I^-} |a_j| \\
\sum_{i \in P^+} a_i - \sum_{j \in I^- \setminus P^-} |a_j| \quad &< b \\
\sum_{i \in P^+} a_i + \sum_{j \in I^- \setminus P^-} a_j \quad &< b \\
\sum_{i \in P^+ \cup I^- \setminus P^-} a_i \quad &< b.
\end{aligned}$$

For $\delta := b - \mathbf{a}(P^+ \cup (I^- \setminus P^-))$ and $M := \{i \in N \setminus (P^+ \cup P^-) \ : \ |a_i| > \delta\}$, the corresponding pack inequality can be expressed as

$$\begin{aligned}
\sum_{i \in M \cap I^+} x_i + \sum_{j \in M \cap I^-} \bar{x}_j \leq 0 \\
\sum_{i \in M \cap I^+} x_i + \sum_{j \in M \cap I^-} (1 - x_j) \leq 0 \\
\sum_{i \in M \cap I^+} x_i + |M \cap I^-| \leq \sum_{j \in M \cap I^-} x_j \\
\sum_{i \in M \cap I^-} x_i - \sum_{j \in M \cap I^+} x_j \geq |M \cap I^-|.
\end{aligned}$$

Proposition 3.23. *The* generalized pack inequality

$$\mathbf{x}(M \cap I^-) - \mathbf{x}(M \cap I^+) \geq |M \cap I^-| \tag{3.27}$$

is valid for $\operatorname{conv}(K_{P^+ \cup P^-})$*. Furthermore, inequality* (3.27) *defines a facet for* $\operatorname{conv}(K_{P^+ \cup P^-})$ *if and only if* $P^+ \cup P^-$ *is of maximal cardinality, i.e.*

$$|a_i| > \delta, \quad \forall\, i \in N \setminus (P^+ \cup P^-)$$

or $M = N \setminus (P^+ \cup P^-)$.

In addition, attributing to the above preliminaries we can rewrite the weight inequalities for the generalized $0-1$ knapsack.

Proposition 3.24. *The generalized weight inequality*

$$\sum_{i\in P^-} a_i x_i - \sum_{i\in P^+} a_i(1-x_i) + \sum_{j\in M\cap I^+} (a_j-\delta)^+ x_j + \sum_{j\in M\cap I^-} (-a_j-\delta)^+(1-x_j) \le 0 \tag{3.28}$$

is valid for $\mathrm{conv}(K)$.

For $\overline{P} = \overline{P}^+ \cup \overline{P}^-$ maximal and corresponding residue $\bar{\delta} = b - \mathbf{a}(\overline{P}^+ \cup (I^- \setminus \overline{P}^-))$, we have the maximal pack inequality

$$\mathbf{x}(I^- \setminus \overline{P}) - \mathbf{x}(I^+ \setminus \overline{P}) \ge |I^- \setminus \overline{P}|. \tag{3.29}$$

and the maximal weight inequality

$$\sum_{i\in P^-} a_i x_i - \sum_{i\in P^+} a_i(1-x_i) + \sum_{j\in I^+\setminus P^+} (a_j-\bar{\delta})^+ x_j + \sum_{j\in I^-\setminus P^-} (-a_j-\bar{\delta})^+(1-x_j) \le 0. \tag{3.30}$$

It can also be seen that the corresponding generalized lifted pack inequality for $\overline{P}$ maximal, can be represented as

$$\begin{aligned}
&\mathbf{x}(I^- \setminus \overline{P}) - \sum_{i\in \overline{P}^+} \alpha_i(1-x_i) - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j\in \overline{P}^-} \alpha_j(1-\bar{x}_j) \ge |I^- \setminus \overline{P}| \\
&\mathbf{x}(I^- \setminus \overline{P}) + \sum_{i\in \overline{P}^+} \alpha_i x_i - \boldsymbol{\alpha}(\overline{P}^+) - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j\in \overline{P}^-} \alpha_j x_j \ge |I^- \setminus \overline{P}| \\
&\mathbf{x}(I^- \setminus \overline{P}) + \sum_{i\in \overline{P}^+} \alpha_i x_i - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j\in \overline{P}^-} \alpha_j x_j \ge |I^- \setminus \overline{P}| + \boldsymbol{\alpha}(\overline{P}^+)
\end{aligned}$$

which yields the generalized lifted pack inequality

$$\mathbf{x}(I^- \setminus \overline{P}) + \sum_{i\in \overline{P}^+} \alpha_i x_i - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j\in \overline{P}^-} \alpha_j x_j \ge |I^- \setminus \overline{P}| + \boldsymbol{\alpha}(\overline{P}^+), \tag{3.31}$$

where α_i, $i \in \overline{P}^+ := \overline{P} \cap I^+$ and α_j, $j \in \overline{P}^- := \overline{P} \cap I^-$ are the corresponding lifting coefficients. Let E be a set of all such indices, i.e. $E := \{i \in \overline{P} \ : \ \alpha_i \ge 1\}$.

We characterize the extension set E with respect to $(\overline{P}^+ \cup \overline{P}^-)$ as

$$E := \left\{ i \in \overline{P} \ : \ |a_i| + \bar{\delta} \ge \max_{j\in N\setminus \overline{P}} |a_j| \right\}, \tag{3.32}$$

where $\bar{\delta} = b - \mathbf{a}(\overline{P}^{+} \cup (I^{-} \setminus \overline{P}^{-}))$.

Further define subsets E^+ and E^- as

$$E^+ := I^+ \cap E \quad E^- := I^- \cap E.$$

The *generalized pack inequality* can now be expressed as

$$\mathbf{x}(E^+ \cup I^- \setminus \overline{P}) - \mathbf{x}(E^- \cup I^+ \setminus \overline{P}) \geq |I^- \setminus \overline{P}| + |E^+|.$$

Proposition 3.25. *The generalized extended pack inequality*

$$\mathbf{x}(E^+ \cup I^- \setminus \overline{P}) - \mathbf{x}(E^- \cup I^+ \setminus \overline{P}) \geq |I^- \setminus \overline{P}| + |E^+|. \tag{3.33}$$

is valid for $\mathrm{conv}(K_{\overline{P}^{+} \cup \overline{P}^{-} \setminus (E^{+} \cup E^{-})})$. *In addition,* (3.33) *defines a facet of* $\mathrm{conv}(K_{\overline{P}^{+} \cup \overline{P}^{-} \setminus (E^{+} \cup E^{-})})$ *if and only if* $\overline{P}$ *is of maximal cardinality and* $\forall\, i \in E\ \exists$ *distinct* $\{j,k\} \in N \setminus \overline{P}$ *such that* $|\mathbf{a}|(\overline{P} \cup \{j,k\} \setminus \{i\}) > b + |\mathbf{a}|(I^-)$.

The extended pack inequalities are often valid for low dimensional extensions of the knapsack set and not the original set itself. Lifting the pack inequalities yields us strong inequalities that are valid for the convex hull of the original knapsack set, $\mathrm{conv}(K)$. The lifted pack inequality for the generalized linear $0-1$ knapsack can be expressed as (3.31)

$$\mathbf{x}(I^- \setminus \overline{P}) + \sum_{i \in \overline{P}^+} \alpha_i x_i - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j \in \overline{P}^-} \alpha_j x_j \geq |I^- \setminus \overline{P}| + \boldsymbol{\alpha}(\overline{P}^+),$$

where $\overline{P}$ represents a maximal pack, and $\alpha_i \geq 0$, $i \in \overline{P}^+$ and $\alpha_j \geq 0$, $j \in \overline{P}^-$ are the corresponding lifting coefficients.

Sequence independent bounds on the aforementioned lifting coefficients can be obtained as a direct generalizations of Proposition 3.14.

Proposition 3.26. *Suppose that* $\overline{P} \subseteq N$ *is a maximal pack. Let* $m = |N \setminus \overline{P}|$ *and suppose the lifted pack inequality* (3.13) *defines a* $n-m-1$ *dimensional face of* $\mathrm{conv}(K)$*, then the following statements hold for all* α_j, $j \in \overline{P}$.

(i) $\alpha_j \leq h$, *if* $|a_j| \leq \overline{A}_h$,

(ii) $\alpha_j \geq h$, *if* $|a_j| \geq \overline{B}_h - \bar{\delta}$,

where $\overline{A}_h = \min\left\{\mathbf{a}(T) \ :\ T \subseteq N \setminus \overline{P},\, |T| = h\right\}$ *and* $\overline{B}_h = \max\left\{\mathbf{a}(T) \ :\ T \subseteq N \setminus \overline{P},\, |T| = h\right\}$ *for* $h = 0, 1, 2, \ldots, m$ *and the excess* $\bar{\delta} = b - \mathbf{a}(\overline{P}^+ \cup (I^+ \setminus \overline{P}^-))$.

Corollary 3.4. *The extended generalized pack inequality*

$$\mathbf{x}(I^- \setminus \overline{P}) + \sum_{i \in \overline{P}^+} c_i x_i - \mathbf{x}(I^+ \setminus \overline{P}) - \sum_{j \in \overline{P}^-} c_j x_j \geq |I^- \setminus \overline{P}| + \mathbf{c}(\overline{P}^+) \tag{3.34}$$

is valid for $\mathrm{conv}(K)$*, where* $c_j = h$, *if* $\overline{A}_h \leq a_j \leq \overline{B}_h - \bar{\delta}$, $j \in \overline{P}$.

3.3 General Submodular Knapsack Polytope

In this section we will extend the results of the $0-1$ linear knapsack to submodular knapsacks. Consider a set function $f : \{0,1\}^n \mapsto \mathbb{R}$, $f(\emptyset) = 0$. For f submodular on a finite set N and $b \in \mathbb{R}$, we define the submodular knapsack set K_f as lower level set of f

$$K_f = \{\mathbf{x} \in \{0,1\}^n \ : \ f(\mathbf{x}) \leq b\}.$$

Special cases for the submodular knapsack polytope, namely when f is non-decreasing on N and when f is non-increasing have been studied by Atamtürk and Narayanan [12] and Atamtürk and Bhardwaj [8] respectively, where they derive valid cover/pack inequalities and their extensions for this special case. The generalization of cover inequalities to this special case, although interesting appears to lack the understanding of their *evolution*. It also appears that the general submodular knapsack has not been studied yet in the literature. In this particular section we will present the corresponding valid inequalities and their extensions for the generalized submodular polytope $\text{conv}(K_f)$, whilst also providing an understanding *vis-à-vis* how these inequalities can be derived from the conjunction of two of the main understandings for knapsacks and submodular functions, namely the cover inequalities and the extended polymatroids. These inequalities per our understanding serve as the most generalized version of the cover and pack inequalities for the knapsack polytope.

3.3.1 Submodular Functions and Extended Polymatroids

Let $N := \{1, \ldots, n\}$ be a finite set and $f : 2^N \to \mathbb{R}$ be a set function on N. Assume without loss of generality that $f(\emptyset) = 0$ since f can be translated otherwise. Define the convex lower envelope of f as

$$P_f := \text{conv}\{(\mathbf{x}, z) \in \{0,1\}^n \times \mathbb{R} \ : \ f(\mathbf{x}) \leq z\}.$$

Observe that P_f is a polyhedron since it is the convex hull of disjunction of 2^n polyhedra obtained for each assignment of $\mathbf{x} \in \{0,1\}^n$.

Definition 3.4. We define a bijection $\boldsymbol{\sigma} : S \subseteq N \mapsto \{1, 2, \ldots, |S|\}$ called a labeling of S and σ_i is the corresponding label of $i \in S$. We define the inverse function of $\boldsymbol{\sigma}$ with $\boldsymbol{\pi}$ and refer to $\boldsymbol{\pi} = \{\pi_1, \pi_2, \ldots, \pi_{|S|}\}$ as a permutation (ordering) of S.

Definition 3.5. For $S \subseteq N$, we define $\mathcal{O}_S$ as the set of all labelings of the set S.

Definition 3.6. For a set function f on N satisfying $f(\emptyset) = 0$, define

$$EP_f := \{\mathbf{v} \in \mathbb{R}^n \ : \ \mathbf{v}(S) \leq f(S) \text{ for all } S \subseteq N\}.$$

The next simple proposition shows a polarity relationship between EP_f and a subset of the valid inequalities for P_f.

Proposition 3.27. (Atamtürk and Narayanan, 2008, [11]) *Inequality* $\mathbf{v}^\top \mathbf{x} \leq z$ *is valid for* P_f *if and only if* $\mathbf{v} \in EP_f$.

Proposition 3.31 also implies the following result:

Proposition 3.28. (Atamtürk and Narayanan, 2008, [11]) *Inequality* $\mathbf{v}^\top \mathbf{x} \leq z$ *is facet-defining for* P_f *if and only if* $\mathbf{v}$ *is an extreme point of* EP_f.

If f is a submodular function, EP_f is called the *extended polymatroid* associated with f [80]. Edmonds [36] characterized the extreme points of the extended polymatroid EP_f.

Theorem 3.1. (Edmonds, 1970, [36]) *For any submodular function* f *on a finite set* N ($f(\emptyset) = 0$), *the vertices of the extended polymatroid* EP_f *are given by*

$$v_{\pi_j} = f(\{\pi_1, \pi_2, \ldots, \pi_j\}) - f(\{\pi_1, \pi_2, \ldots, \pi_{j-1}\}),$$

for a permutation $\boldsymbol{\pi}$ *of* N. *We denote the vertex of* EP_f *corresponding to* $\boldsymbol{\pi}$ *as* $\mathbf{v}^{\boldsymbol{\pi}}$.

We refer to inequalities $\mathbf{v}^\top \mathbf{x} \leq z$ defined by the extreme points of the extended polymatroid EP_f as the *extended polymatroid inequalities.*

Definition 3.7. Let $\mathbf{V}_f$ denote the set of all extreme points of EP_f.

Definition 3.8. For $b \in \mathbb{R}$ define

$$K_{\mathbf{v}} := \left\{\mathbf{x} \in \{0,1\}^n \ : \ \mathbf{v}^\top \mathbf{x} \leq b\right\} \text{ for some } \mathbf{v} \in \mathbf{V}_f \text{ and } K_f := \{\mathbf{x} \in \{0,1\}^n \ : \ f(\mathbf{x}) \leq b\}.$$

Proposition 3.29. $K_f \subseteq K_{\mathbf{v}}$ *for all* $\mathbf{v} \in \mathbf{V}_f$.

Proof. Suppose that $\mathbf{x} \in K_f$. Then, $\mathbf{v}^\top \mathbf{x} \leq f(\mathbf{x}) \leq b$ for all $\mathbf{v} \in \mathbf{V}_f$. Thus, $\mathbf{x} \in K_{\mathbf{v}}$ for all $\mathbf{v} \in \mathbf{V}_f$. □

Proposition 3.30. $\bigcap_{\mathbf{v} \in \mathbf{V}_f} K_{\mathbf{v}} = K_f$.

Proof. It follows from Proposition 3.29 that $K_{\mathbf{v}} \supseteq K_f$ for all $\mathbf{v} \in \mathbf{V}_f$. It follows that $\bigcap_{\mathbf{v} \in \mathbf{V}_f} K_{\mathbf{v}} \supseteq K_f$.

To see the containment $\bigcap_{\mathbf{v} \in \mathbf{V}_f} K_{\mathbf{v}} \subseteq K_f$, suppose that $\mathbf{x} \in \bigcap_{\mathbf{v} \in \mathbf{V}_f} K_{\mathbf{v}}$. Then, by Corollary 44.3e of Schrijver [80], we see that there exists $\bar{\mathbf{v}} \in \mathbf{V}_f$ such that $f(\mathbf{x}) = \bar{\mathbf{v}}^\top \mathbf{x}$, and hence, $f(\mathbf{x}) \leq b$. □

Proposition 3.31. *If* $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$, *is valid for* $K_{\mathbf{v}}$ *for some* $\mathbf{v} \in \mathbf{V}_f$ *then* $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ *is valid for* K_f.

Proof. Proposition 3.29 implies that for $\mathbf{v} \in \mathbf{V}_f$, $K_{\mathbf{v}} \subseteq K_f$. Since $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ is valid for $K_{\mathbf{v}} \supseteq K_f$, it is valid for $\text{conv}(K_f)$. □

Proposition 3.32. *Let $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ be valid $K_{\bar{\mathbf{v}}}$, for some $\bar{\mathbf{v}} \in \mathbf{V}_f$ and $\exists\ \mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^k$, k $(\leq n)$ affinely independent points on the hyperplane $\boldsymbol{\alpha}^\top \mathbf{x} = \beta$ satisfying $f(\mathbf{x}^i) \leq b$ for all $1 \leq i \leq k$ then $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a $k-1$ dimensional face of* $\text{conv}(K_f)$ *if and only if $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a $k-1$ dimensional face of* $\text{conv}(K_{\bar{\mathbf{v}}})$*. In particular, when $k = n$, $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ then defines a facet of both* $\text{conv}(K_{\bar{\mathbf{v}}})$ *and* $\text{conv}(K_f)$*.*

Proof. Sufficiency follows from the validity of $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ for $K_{\bar{\mathbf{v}}}$ and hence K_f. Since $\exists$ $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^k$, k $(\leq n)$ affinely independent points on the hyperplane $\boldsymbol{\alpha}^\top \mathbf{x} = \beta$ satisfying $f(\mathbf{x}^i) \leq b$ for all $1 \leq i \leq k$ thus $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a $k-1$ dimensional face of $\text{conv}(K_f)$.

To see the necessity, observe that since $\mathbf{x}^i$, $1 \leq i \leq k$ are on the hyperplane $\boldsymbol{\alpha}^\top \mathbf{x} = \beta$ satisfying $f(\mathbf{x}^i) \leq b$, it follows from Proposition 3.29 that $\mathbf{x}^i \in K_{\bar{\mathbf{v}}}$. Since $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ is valid $K_{\bar{\mathbf{v}}}$ it follows that $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a $k-1$ dimensional face of $\text{conv}(K_{\bar{\mathbf{v}}})$.

In particular, when $k = n$, $\boldsymbol{\alpha}^\top \mathbf{x} \leq \beta$ defines a $n-1$ dimensional face (facet) of both $\text{conv}(K_f)$ and $\text{conv}(K_{\bar{\mathbf{v}}})$. □

3.3.2 Polyhedral Analysis of K_f

In this section we analyze the polyhedral structure of K_f. Specifically, we derive valid inequalities for K_f and conditions under which these valid inequalities are facet defining. As earlier, let $f : \{0,1\}^n \mapsto \mathbb{R}$ be a submodular set function on a finite set N. Assume without loss of generality $f(\emptyset) = 0$. Furthermore, we assume $\min\limits_{S \subseteq N \setminus i} f(S) \leq b$ for all $i \in N$. Define the sets, I^+ and I^- as

$$I^+ = \{i \in N \ : \ \rho_i(N \setminus i) > 0\}. \tag{3.35}$$
$$I^- = \{j \in N \ : \ \rho_i(\emptyset) < 0\}. \tag{3.36}$$

Observe that for $\sum_{i \in S} v_{\pi_i} = f(S)$ irrespective of the ordering $\boldsymbol{\pi}$ of the elements of N. For the permutation $\boldsymbol{\pi}$, define the index sets $I_{\boldsymbol{\pi}}$ and $J_{\boldsymbol{\pi}}$ as following

$$I_{\boldsymbol{\pi}} = \{\pi_i \in \boldsymbol{\pi} \ : \ v_{\pi_i} > 0\}. \tag{3.37}$$
$$J_{\boldsymbol{\pi}} = \{\pi_j \in \boldsymbol{\pi} \ : \ v_{\pi_i} < 0\}. \tag{3.38}$$

One can easily observe that $I^+ \subseteq I_{\boldsymbol{\pi}}$ and $I^- \subseteq J_{\boldsymbol{\pi}}$. In particular, $I^+ = \bigcap\limits_{\boldsymbol{\pi} \in \mathbf{V}_f} I_{\boldsymbol{\pi}}$ and $I^- = \bigcap\limits_{\boldsymbol{\pi} \in \mathbf{V}_f} J_{\boldsymbol{\pi}}$.

3.3.3 Valid Inequalities for K_f

We begin our subsequent discussion on valid inequalities for K_f by presenting the results on the trivial facets of the K_f.

Proposition 3.33. *Inequality $x_i \geq 0$, $i \in I^+$ defines a non-empty face of* $\operatorname{conv}(K_f)$.

Proof. Consider for permutation $\boldsymbol{\pi}$ the corresponding set $I_{\boldsymbol{\pi}}$ as defined in (3.37). $x_i \geq 0$, $i \in I_{\boldsymbol{\pi}}$ is facet defining for $K_{\mathbf{v}^{\boldsymbol{\pi}}}$. Let $\mathcal{S} = \left\{ S_i \;:\; S_i = \arg\min_{S \subseteq N \setminus i} f(S) \leq b,\; i \in I^+ \right\}$. Observe that $|\mathcal{S}| \geq 1$ since $\min_{S \subseteq N \setminus i} f(S) \leq b$ for all $i \in N$. Thus there is at least one point $\mathbf{x}_S$, $S \in \mathcal{S}$ such that $f(\mathbf{x}_S) \leq b$ on the face $x_i = 0$, $i \in I^+$. The result follows. □

Proposition 3.34. *Inequality $x_i \leq 1$, $i \in I^-$ defines a non-empty face of* $\operatorname{conv}(K_f)$.

Proof. Consider for permutation $\boldsymbol{\pi}$ the corresponding set $J_{\boldsymbol{\pi}}$ as defined in (3.38). $x_i \leq 1$, $i \in J_{\boldsymbol{\pi}}$ is facet defining for $K_{\mathbf{v}^{\boldsymbol{\pi}}}$. Let $\mathcal{S} = \left\{ S_i \;:\; S_i = \arg\min_{S \subseteq N \setminus i} f(S) \leq b,\; i \in I^- \right\}$. Observe that $f(S \cup i) \leq b$ for all $S \in \mathcal{S},\; i \in I^-$. Furthermore, see that $|\mathcal{S}| \geq 1$ since $\min_{S \subseteq N \setminus i} f(S) \leq b$ for all $i \in N$. Thus there is at least one point $\mathbf{x}_S$, $S \in \mathcal{S}$ such that $f(\mathbf{x}_S) \leq b$ on the face $x_i = 1$, $i \in I^-$. The result follows. □

We now present the notion of submodular covers analogous to linear $0-1$ knapsack covers as discussed in Section 3.2.3.

3.3.4 Submodular Cover Inequalities

Definition 3.9. $S \subseteq N$ is a *submodular cover* if $f(S) > b$ with excess $\lambda := f(S) - b > 0$.

In particular, submodular covers are the sets that are infeasible for K_f. Valid inequalities from this characterization follow immediately.

Proposition 3.35. *For a submodular cover $S \subseteq N$ the cover inequality*

$$\mathbf{x}(S) - \mathbf{x}(N \setminus S) \leq |S| - 1 \tag{3.39}$$

is valid for K_f.

Proof. Define $\overline{K_f} := \{\mathbf{x} \in \{0,1\}^n \;:\; \mathbf{x}(S) - \mathbf{x}(N \setminus S) \geq |S|\}$. It suffices to show that $f(\mathbf{x}) > b,\; \forall\, \mathbf{x} \in \overline{K_f}$. It is easy to see that $\overline{K_f} = \{\mathbf{x} \in \{0,1\}^n \;:\; x_i = 1\; \forall\, i \in S,\; x_i = 0\; \forall\, i \in N \setminus S\}$. The result follows from Definition 3.9. □

A close observation yields that the cover inequalities (3.39) are weak. In the following discussion we will propose strong inequalities for the lower dimensional restrictions of K_f. Throughout the rest of the discussion we assume, without lost of generality, that $\rho_i(S \setminus i) > 0$ $\forall i \in S$.

Definition 3.10. For $S_1, S_2 \subseteq N$, we define a restriction of K_f as

$$K_f(S_1, S_2) = \{\mathbf{x} \in K_f \ : \ x_i = 1 \text{ for all } i \in S_1, \, x_j = 0 \text{ for all } j \in S_2\}.$$

Valid inequalities for this restriction follow from the characterization of submodular covers immediately.

Proposition 3.36. *For a submodular cover $S \subseteq N$ the cover inequality*

$$\mathbf{x}(S) \leq |S| - 1 \tag{3.40}$$

is valid for $\text{conv}(K_f(\emptyset, N \setminus S))$. *In addition,* (3.40) *defines a facet of* $\text{conv}(K_f(\emptyset, N \setminus S))$ *if and only if $f(S \setminus i) \leq b$ for all $i \in S$.*

Proof. Consider $\overline{K}_f(S) := \{\mathbf{x} \in K_f(\emptyset, N \setminus S) \ : \ \mathbf{x}(S) \geq |S|\}$. It is easy to see that $\overline{K}_f(S) = \emptyset$ since S is a cover. For the second part consider the $|S|$ affinely independent points $\mathbb{1} - \mathbf{e}_i \in K_f(\emptyset, N \setminus S)$ for $0 \leq i \leq |S|$ on the face $\mathbf{x}(S) = |S| - 1$. Conversely, assume $\exists\, i \in S$ such that $f(S \setminus i) > b$. The valid cover inequality

$$\mathbf{x}(S \setminus i) \leq |S \setminus i| - 1$$

and $x_i \leq 1$ dominate inequality (3.40). □

Definition 3.11. For a cover $S \subseteq N$ define the index set

$$\bar{S} := \{j \in N \setminus S \ : \ \rho_j(N \setminus j) < 0\}.$$

Proposition 3.37. *For a submodular cover $S \subseteq N$, the submodular cover inequality*

$$\mathbf{x}(S) - \mathbf{x}(\bar{S}) \leq |S| - 1 \tag{3.41}$$

is valid for $\text{conv}(K_f)$. *In addition,* (3.41) *is facet defining for* $\text{conv}(K_f(\emptyset, N \setminus (S \cup \bar{S})))$ *only if*

$$f(S \setminus i) \leq b \ \ \forall\, i \in S \text{ and}$$
$$f(S \cup j) \leq b \ \ \forall\, j \in \bar{S},$$

Proof. Define $\overline{K_f} := \{\mathbf{x} \in \{0,1\}^n \,:\, \mathbf{x}(S) - \mathbf{x}(\bar{S}) \geq |S|\}$. It suffices to show that $f(\mathbf{x}) > b,\ \forall \mathbf{x} \in \overline{K_f}$. It is easy to see that $\overline{K_f} = \{\mathbf{x} \in \{0,1\}^n \,:\, x_i = 1\ \forall i \in S,\ x_i = 0\ \forall i \in \bar{S}\}$. Since $\rho_j(N \setminus j) \geq 0\ \forall\, j \in N \setminus (S \cup \bar{S})$, $f(S \cup T) > b\ \forall\, T \subseteq N \setminus (S \cup \bar{S})$. The result follows.

For the second part consider the $|S| + |\bar{S}|$ points $\mathbf{x}^k \in \{0,1\}^n$ defined as

$$\begin{aligned} \mathbf{x}^k &= (\mathbb{1} - \mathbf{e}_k, \mathbf{0}) \quad \forall\, k \in S, \\ \mathbf{x}^k &= (\mathbb{1}, \mathbf{e}_k) \qquad\quad \forall\, k \in \bar{S}. \end{aligned}$$

The $|S| + |\bar{S}|$ points defined above are affinely independent. Since

$$\begin{aligned} f(S \setminus i) &\leq b \quad \forall\, i \in S \text{ and} \\ f(S \cup j) &\leq b \quad \forall\, j \in \bar{S}, \end{aligned}$$

$\mathbf{x}^k \in \text{conv}(K_f(\emptyset, N \setminus (S \cup \bar{S})))$ and lie on the face $\mathbf{x}(S) - \mathbf{x}(\bar{S}) = |S| - 1$. □

Remark 3.1. In the special case when $\bar{S} = \emptyset$ i.e. f is non decreasing on N, inequality (3.41) yields the cover inequalities considered in [12]. When $S = \emptyset$ i.e. f is non increasing on N, inequality (3.41) yields the pack inequalities discussed in [8] (Chapter 2). Proposition 3.37 thus generalizes the results of Atamtürk and Narayanan [12] and Atamtürk and Bhardwaj [8] for monotone submodular set functions.

In the special case when $\bar{S} \setminus \{j \in N \setminus S \,:\, \rho_j(S) \leq -\lambda\} = \emptyset$, we can further strengthen the result of Proposition 3.37.

Proposition 3.38. *If* $\bar{S} \setminus \{j \in N \setminus S \,:\, \rho_j(S) \leq -\lambda\} = \emptyset$ *then* (3.41) *is facet defining for* $\text{conv}(K_f(\emptyset, N \setminus (S \cup \bar{S})))$ *if and only if* $f(S \setminus i) \leq b \ \ \forall\, i \in S$.

Proof. Necessity follows from Proposition 3.37. To observe sufficiency observe that if $\exists\, i \in S$ such that $f(S \setminus i) > b$ then the valid submodular cover inequality

$$\mathbf{x}(S \setminus i) - \mathbf{x}(\bar{S}) \leq |S \setminus i| - 1$$

and $x_i \leq 1$ dominate inequality (3.41). □

Example 3.1. Consider the set K defined as

$$K = \left\{\mathbf{x} \in \{0,1\}^3 \,:\, 2x_1^2 + x_2^2 + 2x_3^2 - x_1x_2 - 2x_1x_3 - 4x_2x_3 \leq 1\right\}.$$

The set K can be enumerated as $K = \{(0,0,0), (0,1,0), (0,1,1), (1,1,1)\}$.

For strong submodular cover $S = \{1\}$ and $T = \{2,\, 3\}$, we write the submodular cover inequality

$$x_1 \leq x_2 + x_3.$$

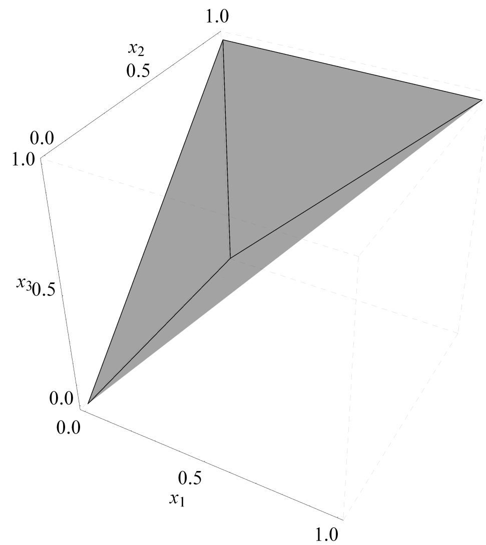


Figure 3.2: Convex hull $conv(K)$

For strong submodular cover $S = \{3\} : T = \{1, 2\}$, submodular cover inequality

$$x_3 \leq x_1 + x_2.$$

Both inequalities define facets of $\text{conv}(K)$.

Proposition 3.36 and Proposition 3.37 provide conditions under which the corresponding cover and submodular cover inequalities are valid and facet defining for the restrictions of K_f. These conditions, however, are not sufficient for the corresponding inequalities to be facet defining for K_f itself. An approach to derive strong inequalities for K_f is to study the lower dimensional projections of K_f and derive strong valid inequalities for these projections and lift the same to original variable space.

Proposition 3.37 provides necessary conditions to derive strong valid inequalities for low dimensional restrictions of K_f. These inequalities can then be lifted to yield strong valid inequalities in the original space. Lifting, and in particular, sequential lifting to obtain exact lifting coefficients can be computationally expensive. In Section 3.4 we present efficient ways to lift the low dimensional restrictions of K_f via the extended polymatroids associated with the set function f.

3.3.5 Submodular Pack Inequalities

With apropos to the preliminaries defined in Section 3.3.4, we define the notion of *submodular packs*

Definition 3.12. $P \subseteq N$ is a *submodular pack* if $f(P) < b$ with residual $\delta := b - f(P) > 0$.

For a submodular pack $P \subseteq N$, define the index set $P^+ := \{i \in I^+ \setminus P \ : \ \rho_i(P) > \delta\}$. The following result is an immediate consequence.

Proposition 3.39. *For a submodular pack $P \subseteq N$, the submodular pack inequality*

$$\mathbf{x}(P^+) \leq 0 \tag{3.42}$$

is valid for $K_f(P, N \setminus (P \cup I^+))$.

Observe that, given any pack $P \subseteq N$, it is trivial to introduce elements from the complement set $N \setminus P$ to obtain a pack $\overline{P}$ such that $\overline{P}^+ = I^+ \setminus \overline{P}$. This observation can be used to further strengthen submodular pack inequalities.

Proposition 3.40. *For a submodular pack $P \subseteq N$ such that $P^+ = I^+ \setminus P$, the submodular pack inequality* (3.42) *defines a facet of $K_f(P, N \setminus (P \cup I^+))$.*

Submodular pack inequalities (3.42) are derived from the restrictions of the submodular knapsack polytope and are valid for the corresponding projections and not necessarily for K_f. Weight inequalities [94] as seen in Sections 3.2.2 and 3.2.3 that are valid for the knapsack set, can be directly generalized to the case of submodular knapsack *via* extended polymatroid associated with the corresponding set function f. We formalize this in the following result.

Proposition 3.41. *The submodular weight inequality*

$$\sum_{j \in J_{\boldsymbol{\pi}} \setminus P} \rho_j(N \setminus j) x_j - \sum_{i \in P \cap I_{\boldsymbol{\pi}}} f(i)(1 - x_i) + \sum_{i \in I_{\boldsymbol{\pi}} \setminus P} (\rho_i(N \setminus i) - \delta)^+ x_i + \sum_{j \in P \cap J_{\boldsymbol{\pi}}} (-f(j) - \delta)^+ (1 - x_j) \leq 0$$

is valid for K_f, where $P \subseteq N$ is a pack and $\delta = b - f(P)$.

Proof. Consider a permutation $\boldsymbol{\pi} = \{1, 2, \ldots, n\}$ of the elements of the index set N. Define the corresponding index sets $I_{\boldsymbol{\pi}}$ and $J_{\boldsymbol{\pi}}$. Proposition 3.24 suggests that the following weight inequality

$$\sum_{j \in J_{\boldsymbol{\pi}} \setminus P} v_j^{\boldsymbol{\pi}} x_j - \sum_{i \in P \cap I_{\boldsymbol{\pi}}} v_i^{\boldsymbol{\pi}} (1 - x_i) + \sum_{i \in I_{\boldsymbol{\pi}} \setminus P} (v_i^{\boldsymbol{\pi}} - \bar{\delta})^+ x_i + \sum_{j \in P \cap J_{\boldsymbol{\pi}}} (-v_j^{\boldsymbol{\pi}} - \bar{\delta})^+ (1 - x_j) \leq 0$$

is valid for K_f. Furthermore, submodularity of the set function f suggests

$$\rho_j(N \setminus j) \leq v_j^{\boldsymbol{\pi}} \leq f(j), \forall \ j \in N, \ \forall \ \boldsymbol{\pi}.$$

The result follows. $\square$

3.3.6 Lifted Submodular Cover Inequalities

In this section we study the lifting problem of the valid inequalities discussed earlier in order to strengthen them. The lifting procedure has been very effective in strengthening inequalities for the linear $0-1$ min-knapsack set [15, 17, 18, 43, 45, 95] as described in Section 3.2.1. The lifting problem for the submodular cover inequalities for K_f is itself an optimization problem over the submodular knapsack set.

In particular, we lift the submodular cover inequality (3.41) to a valid inequality of the form,

$$\mathbf{x}(S) - \mathbf{x}(\overline{S}) + \sum_{i \in I_{\boldsymbol{\pi}} \setminus S} \alpha_i x_i - \sum_{j \in J_{\boldsymbol{\pi}} \setminus \overline{S}} \alpha_j x_j \leq |S| - (\boldsymbol{\alpha}(J_{\boldsymbol{\pi}} \setminus \overline{S}) + 1) \tag{3.43}$$

where $\alpha_i \geq 0$, $i \in N \setminus (S \cup \overline{S})$ are the corresponding lifting coefficients. Observe that unlike in the linear $0-1$ knapsack case, the lifted cover inequalities are dependent on the sequence $\boldsymbol{\pi}$ used for lifting.

3.3.7 Strengthening the Valid Inequalities *via* Extensions

As in the case of linear $0-1$ knapsack, we can strengthen the inequalities corresponding to *submodular covers* (3.39) via computationally efficient extensions. In the following discussion we provide an analogous procedure to extend these inequalities as in Section 3.2.1.

Definition 3.13. For a submodular cover $S \subsetneq N$ and $\overline{S} = \{j \in N \setminus S \ : \ \rho_j(N \setminus j) < 0\}$ let $\boldsymbol{\pi}$ be a permutation of elements of $N \setminus (S \cup \overline{S})$. Define $S_k := S_{k-1} \cup (k)$, with $S_0 = S$. Extension of $S \cup \overline{S}$ w.r.t. $\boldsymbol{\pi}$ is defined as

$$E_{\boldsymbol{\pi}}(S) := \left\{ (k) \in \boldsymbol{\pi} \ : \ \rho_{(k)}(S_{k-1}) \geq \max_{j \in (S \cup \overline{S})} \{\rho_j(\emptyset), |\rho_j(N \setminus j)|\} \right\}$$

With apropos to the extension set $E_{\boldsymbol{\pi}}(S)$ we can extend the submodular cover inequalities in the following manner.

Proposition 3.42. *Extended submodular cover inequality*

$$\mathbf{x}(S \cup E_{\boldsymbol{\pi}}(S)) - \mathbf{x}(\overline{S}) \leq |S| - 1 \tag{3.44}$$

is valid for K.

Proof. Let U be a subset of $S \cup E_{\boldsymbol{\pi}}(S)$ and $R \subseteq \overline{S}$ such that $|U| - |R|$ is at least $|S|$. It is sufficient to show $f(U \cup R) > b$. Let $K = S \setminus U$ and $L \subseteq E_{\boldsymbol{\pi}}(S) := \{l_1, l_2, \ldots, l_{|L \setminus R|}, \ldots, l_{|L|}\}$

indexed consistently with $\boldsymbol{\pi}$ such that $U = S \cup L \setminus K$.

$$\begin{aligned}
f(U \cup R) &= f(S \cup L \cup R \setminus K) \\
&= f(S \setminus K) + \sum_{l_i \in L} \rho_{l_i}(S \cup \{l_1, l_2, \dots l_{i-1}\} \setminus K) + \rho_R(S \cup L \setminus K) \\
&= f(S \setminus K) + \sum_{i=1}^{|L \setminus R|} \rho_{l_i}(S \cup \{l_1, l_2, \dots l_{i-1}\} \setminus K) + \\
&\sum_{i=|L \setminus R|+1}^{|L|} \rho_{l_i}(S \cup \{l_{|L \setminus R|+1}, l_{|L \setminus R|+2}, \dots l_{i-1}\} \setminus K) + \rho_R(S \cup L \setminus K) \\
&\geq f(S \setminus K) + \sum_{i=1}^{|L \setminus R|} \rho_{l_i}(S \cup \{l_1, l_2, \dots l_{i-1}\} \setminus K) + \\
&\sum_{i=|L \setminus R|+1}^{|L|} \rho_{l_i}(S \cup \{l_{|L \setminus R|+1}, l_{|L \setminus R|+2}, \dots l_{i-1}\} \setminus K) + \sum_{j \in R} \rho_j(N \setminus j) \\
&\geq f(S \setminus K) + \sum_{(k) \in \boldsymbol{\pi}} \rho_{(k)}(S_{k-1}) \\
&\geq f(S \setminus K) + \sum_{i \in K} \rho_i(\emptyset) \\
&\geq f(S \setminus K) + \sum_{i \in K} \rho_i(S \setminus K) \geq f(S) > b.
\end{aligned}$$

The second inequality follows from the definition of $E_{\boldsymbol{\pi}}(S)$, submodularity of f and the observation that $\rho_j(N \setminus j) \geq 0 \ \forall \ j \in N \setminus (S \cup \overline{S})$. □

Remark 3.2. It should be observed that as in the case of $0-1$ linear knapsack, and stated in Proposition 3.21, the extensions for submodular knapsack are *not* sequence independent.

Remark 3.3. In the special case when $\overline{S} = \emptyset, \forall \boldsymbol{\pi}$ i.e. f is non decreasing on N, inequality (3.44) yields an extension for the case considered in [12].

3.3.8 Sequence Independent Bounds on Lifting Coefficients

Akin to the linear $0-1$ knapsacks, we can derive the sequence independent lifting coefficients for the submodular knapsack K_f. It is now that we will utilize the results from Section 3.2.3 to derive these bounds. In addition we will also demonstrate that the earlier results by Atamtürk and Narayanan [12] are a special case of these generalizations. Before proceeding, we define the following preliminaries.

Definition 3.14. For an index set T, let $\boldsymbol{\sigma}_T = \{1, 2, \dots |T|\}$ be a labeling of elements of T and $\boldsymbol{\pi}_T = \boldsymbol{\sigma}_T^{-1}$ consistent with Definition 3.4. We define the set function $g : \{0,1\}^{|T|} \mapsto \mathbb{R}$

as

$$g(\boldsymbol{\pi}_T) = \sum_{i=1}^{|T|} |\rho_{\pi_i}(\{\pi_1, \pi_2, \ldots, \pi_{i-1}\})| . \tag{3.45}$$

Observe that when f is monotone non-decreasing (non-increasing) then $g(\boldsymbol{\pi}_T)$ is independent of the permutation $\boldsymbol{\pi}_T$ and evaluates to $f(T)$ $(-f(T))$.

Definition 3.15. For $h \geq 0$, we define

$$A_h := \max \left\{ g(\boldsymbol{\pi}_T) \ : \ T \subseteq S \cup \overline{S}, \ |T| = h, \ \boldsymbol{\pi}_T = \boldsymbol{\sigma}_T^{-1}, \ \forall \ \boldsymbol{\sigma}_T \in \mathcal{O}_T \right\}, \tag{3.46}$$

$$B_h := \min \left\{ g(\boldsymbol{\pi}_T) \ : \ T \subseteq S \cup \overline{S}, \ |T| = h, \ \boldsymbol{\pi}_T = \boldsymbol{\sigma}_T^{-1}, \ \forall \ \boldsymbol{\sigma}_T \in \mathcal{O}_T \right\}. \tag{3.47}$$

Owing to the above characterizations of A_h and B_h the following results follow from Proposition 3.22 and Proposition 3.31.

Proposition 3.43. *Let the submodular cover inequality* (3.41) *be lifted to a valid inequality of the form* (3.43)*. Then for* $k \in N \setminus (S \cup \overline{S})$

1. $\alpha_k \geq h$, *if* $\min\{|f(k)|, |\rho_k(N \setminus k)|\} \geq A_h$.
2. $\alpha_k \leq h$, *if* $\max\{|f(k)|, |\rho_k(N \setminus k)|\} \leq b - B_{|S \cup \overline{S})|-1-h}$.

Remark 3.4. In the special case when f is non decreasing on N, Proposition 3.43 yields the result of Proposition 7 in [12].

3.4 Lifting *via* Extended Polymatroids

In the previous section we generalized the existing results on monotone submodular knapsacks to general submodular knapsack set. Monotonicity however is an important assumption in this context. To observe this, note that in the case when the underlying submodular function is monotone (non-decreasing/non-increasing) then the coefficients of each extended polymatroid inequality are all non-negative/non-positive. Louveaux and Weismantel [61] showed that in the case of intersection of multiple $0-1$ linear knapsacks constraints, if the coefficient matrix is all non-negative/non-positive then each of the facets for the intersection of the knapsacks can be derived from the individual knapsack constraints. This explains the computational effectiveness of the cover inequalities in the monotone case [12, 8]. The same argument however doesn't extend to the case of general submodular knapsack.

In this section we propose a way to utilize the extended polymatroid inequalities to strengthen the submodular cover inequalities. As a preliminary consider the following,

Definition 3.16. For the extended polymatroid inequality corresponding to a permutation $\boldsymbol{\pi} = \{\pi_1, \pi_2, \ldots, \pi_n\}$ of the index set N, we define an extended polymatroid cover as any cover corresponding to the linear $0-1$ knapsack $\mathbf{v}^{\boldsymbol{\pi}}\mathbf{x} \leq b$, $\mathbf{v}^{\boldsymbol{\pi}} \in \mathbf{V}_f$.

Definition 3.17. Let $S \subseteq N$ be a submodular cover. Also let $\boldsymbol{\sigma}_S = \{1, 2, \ldots |S|\}$ be a labeling of elements of S and $\boldsymbol{\sigma}_{N \setminus S} = \{1, 2, \ldots |N \setminus S|\}$ be a labeling of elements of $N \setminus S$. Define the set

$$\mathcal{P}_S := \left\{ \boldsymbol{\pi} = \{\boldsymbol{\pi}_S, \boldsymbol{\pi}_{N \setminus S}\} \ : \ \boldsymbol{\pi}_S = \boldsymbol{\sigma}_S^{-1} \text{ and } \boldsymbol{\pi}_{N \setminus S} = \boldsymbol{\sigma}_{N \setminus S}^{-1} \text{ for all } \boldsymbol{\sigma}_S \in \mathcal{O}_S, \boldsymbol{\sigma}_{N \setminus S} \in \mathcal{O}_{N \setminus S} \right\}$$

Observe that $|\mathcal{P}_S| = |S|! \times |N \setminus S|!$. The following result serves as a preliminary to derive strong valid inequalities using the extended polymatroid of f.

Proposition 3.44. *For $S \subseteq N$ defining a submodular cover, the submodular cover inequality* (3.41) *is valid for all extended polymatroid inequalities $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x}$, $\boldsymbol{\pi} \in \mathcal{P}_S$.*

Proof. Consider the submodular cover S and the extended polymatroid inequality $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x} \leq b$ corresponding to some $\boldsymbol{\pi} \in \mathcal{P}_S$. The cover inequality

$$\mathbf{x}(S) - \mathbf{x}(J_{\boldsymbol{\pi}}) \leq |S| - 1.$$

is valid for the linear $0-1$ knapsack defined by $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x} \leq b$. Since $J_{\boldsymbol{\pi}} \subseteq \overline{S}$, $\forall\ \boldsymbol{\pi} \in \mathcal{P}_S$, we obtain that

$$\mathbf{x}(S) - \mathbf{x}(\overline{S}) \leq |S| - 1.$$

is valid for $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x} \leq b$, $\boldsymbol{\pi} \in \mathcal{P}_S$. □

Proposition 3.44 suggests a way to utilize the extended polymatroid inequalities to lift the submodular cover inequality. Indeed the submodular cover inequality is valid for the extended polymatroid inequalities for permutations $\boldsymbol{\pi} \in \mathcal{P}_S$. Lifting these inequalities while utilizing information from an aggregation of subset of extended polymatroid inequalities will yield valid inequalities for K_f.

The following example serves as a motivation to consider the aggregation of extended polymatroid inequalities to lift the cover inequalities of the form (3.41).

Example 3.2. Consider the following conic-quadratic knapsack set defined by a submodular set function.

$$X = \left\{ \mathbf{x} \in \{0,1\}^5 \ : \ 2x_1 + 2x_2 + x_3 + x_4 + x_5 + \sqrt{9x_3^2 + 9x_4^2 + 9x_5^2} \leq 3.5 \right\}$$

For submodular cover $= \{1, 2\}$, we can obtain the following extended submodular cover inequalities [12].

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 \qquad &\le 1 \\ x_1 + x_2 + \qquad x_4 + x_5 &\le 1 \\ x_1 + x_2 + x_3 \qquad + x_5 &\le 1 \end{aligned}$$

The corresponding extended polymatroid inequalities are

$$\begin{aligned} 2x_1 + 2x_2 + 4.000x_3 + 2.242x_4 + 1.954x_5 &\le 3.5 \\ 2x_1 + 2x_2 + 2.242x_3 + 1.952x_4 + 4.000x_5 &\le 3.5 \\ 2x_1 + 2x_2 + 1.952x_3 + 4.000x_4 + 2.242x_5 &\le 3.5. \end{aligned}$$

A simple aggregation of the extended polymatroid inequalities yields the aggregated extended polymatroid inequality

$$6x_1 + 6x_2 + 8.196x_3 + 8.196x_4 + 8.196x_5 \le 10.5$$

which yields the extended polymatroid cover inequality,

$$x_1 + x_2 + x_3 + x_4 + x_5 \le 1.$$

The extended polymatroid cover inequality obtained via aggregation of extended polymatroid inequalities dominates each of the extended submodular cover inequalities.

We refer to the inequality obtained by aggregation of extended polymatroid inequalities as the *aggregated extended polymatroid inequality*. Example 3.2 motivates aggregation of extended polymatroid inequalities to derive strong valid inequalities. As employed in the example, a trivial way to aggregate the extended polymatroid inequalities is via simple addition. Once we obtain an aggregated extended polymatroid inequality we can lift the submodular cover inequality (valid for aggregation) using sequence independent lifting techniques for linear $0-1$ knapsacks [43, 42, 44, 7, 17]. We formalize the idea of extended polymatroid aggregation in the following.

For a submodular cover $S \subseteq N$, let $\{\boldsymbol{\pi}_i\}_{1\le i\le m} \subseteq \mathcal{P}_S$ be a set of permutations corresponding to the extended polymatroid inequalities $\mathbf{v}^{\boldsymbol{\pi}_i \top}\mathbf{x} \le b$, $1 \le m$ to be aggregated. Furthermore, let $\mathbf{w} = \{w_1, w_2, \ldots, w_m\}$ such that $\mathbb{1}^\top \mathbf{w} = 1$ be the normalized aggregation weights apropos to the extended polymatroid inequalities. Define $\mathbf{A} = [\mathbf{v}^{\boldsymbol{\pi}_1}, \mathbf{v}^{\boldsymbol{\pi}_2}, \mathbf{v}^{\boldsymbol{\pi}_m}]$ as the matrix with extended polymatroid coefficients. The aggregated extended polymatroid inequality obtained using weights $\mathbf{w}$ is

$$(\mathbf{A}\mathbf{w})^\top \mathbf{x} \le b \tag{3.48}$$

Corollary 3.5. *For $S \subseteq N$ defining a submodular cover, the submodular cover inequality* (3.41) *is valid for the aggregated extended polymatroid inequality* (3.48)*.*

Proof. Proposition 3.44 yields that the submodular cover inequality (3.41) is valid for all extended polymatroid inequalities $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x}$, $\boldsymbol{\pi} \in \mathcal{P}_S$. the submodular cover inequality (3.41) is thus valid for any convex combination of the extended polymatroid inequalities $\mathbf{v}^{\boldsymbol{\pi}\top}\mathbf{x}$ for $\boldsymbol{\pi} \in \mathcal{P}_S$. The result follows. □

The corresponding cover inequality to be lifted is

$$\mathbf{x}(S) - \mathbf{x}(\overline{S}) \leq |S| - 1.$$

Indeed the obvious question regarding the aggregation of extended polymatroid inequalities pertains to deriving aggregation weights $\mathbf{w}$. The problem of finding the *best* aggregation weights to lift the aggregated extended polymatroid inequality depends on the lifting procedure to be used as well. As seen in Example 3.2, one way to lift inequality (3.41) is by using the sequence independent bounds introduced by Balas [17]. These sequence independent bounds on the lifting coefficients have been used to lift cover inequalities using efficiently computable extensions in the case of monotone submodular knapsacks [12, 8]. The problem of finding optimal aggregation weights $\mathbf{w}$ to derive extensions of inequality (3.41) using sequence independent bounds can be formulated as

$$\begin{array}{llrcl} & \text{minimize} & & \mathbb{1}^\top \mathbf{s} & \\ (\text{AEPW}) & \text{subject to} & \displaystyle\sum_{i=|S|+1}^{n} |\mathbf{v}^{\boldsymbol{\pi}_i} w_i| & \geq & (\mathbb{1} - \mathbf{s}) \cdot \alpha \\ & & \mathbb{1}^\top \mathbf{w} & = & 1 \\ & & \mathbf{s} & \in & \{0,1\}^{|N \setminus S|} \\ & & \mathbf{w} & \geq & \mathbf{0} \end{array}$$

where $\alpha = \max_{j \in S \cup \overline{S}} \left(|f(j)| - |\rho_j(N \setminus j)|\right)^+ + |\rho_j(N \setminus j)|$. Let $(\mathbf{s}^*, \mathbf{w}^*)$ denote the optimal solution to (AEPW). The extended submodular cover inequality derived via aggregation of extended polymatroids is

$$\mathbf{x}(S \cup E^+) - \mathbf{x}(\overline{S} \cup E^-) \leq |S| - (|E^-| + 1) \tag{3.49}$$

where $E^+ := \left\{ j \in N \setminus (S \cup \overline{S}) \ : \ (\mathbf{A}\mathbf{w}^*)_j \cdot (1 - s_j^*) > 0 \right\}$ and
$E^- := \left\{ j \in N \setminus (S \cup \overline{S}) \ : \ (\mathbf{A}\mathbf{w}^*)_j \cdot (1 - s_j^*) < 0 \right\}$.

Proposition 3.45. *Finding optimal aggregation weights $\mathbf{w}^*$ to derive extensions of the submodular cover inequality is $\mathcal{NP}$-hard.*

Proof. Finding optimal aggregation weights $\mathbf{w}$ to to derive extensions of the submodular cover inequality is equivalent to finding an optimal solution for (AEPW). (AEPW) is an instance of **MAX-CSP** which is $\mathcal{NP}$-hard. $\square$

Finding optimal aggregation weights in general is computationally expensive. Observe that any feasible solution $(\bar{\mathbf{s}}, \overline{\mathbf{w}})$ can be used to derive a valid lifted submodular cover inequality. In Example 3.2 we utilized equal weights to aggregate the extended polymatroid inequality. Better heuristics can be used to derive good aggregation weights and in turn computationally efficient valid inequalities. As we will see in Section 3.6 even simple heuristics yield substantial computational performance improvement. For the computational analysis we will employ simple addition as an aggregation heuristic.

Observe that deriving extensions of the submodular cover inequality is a very special case of the lifting. In particular, for extended valid inequalities the lifting coefficients are restricted to take values from the set $\{-1, 0, 1\}$. In other words, the primary objective while extending any valid inequality is to establish whether or not a variable currently not present in the valid inequality can be introduced in the inequality with a non-zero lifting coefficient. Indeed, deriving tighter bounds on the exact lifting coefficients with further help strengthen the submodular cover inequalities.

Superadditive lifting techniques have been studied quite extensively with reference to linear $0-1$ knapsacks in literature [43, 42, 44, 7]. This lifting procedure involves deriving superadditive lower bounds on the exact lifting functions to yield sequence independent lifting. We refer the reader to [5] for a survey of sequence independent lifting procedures using superadditive lower bounds. For given weights $\mathbf{w}$, the aggregated extended polymatroid inequality (3.48) can be lifted using the superadditive lifting techniques in the following manner.

Consider a submodular cover $S \subseteq N$. For $\overline{S}$, $\mathbf{A}$ as defined earlier and given aggregation weights $\mathbf{w}$ let $\boldsymbol{\omega} = \mathbf{A}\mathbf{w}$ and define the index sets,

$$\begin{aligned} A^+ &:= \left\{ j \in N \setminus (S \cup \overline{S}) \ : \ \omega_j > 0 \right\} \\ A^- &:= \left\{ j \in N \setminus (S \cup \overline{S}) \ : \ \omega_j < 0 \right\} \end{aligned}$$

Define $L_h = \max \left\{ \sum_{j \in T} |\omega_j| \ : \ T \subseteq (S \cup \overline{S}),\, |T| = h \right\}$.

With the preliminaries defined above we can now derive the *lifted submodular cover inequality*.

Proposition 3.46. *The lifted submodular cover inequality*

$$\mathbf{x}(S) + \sum_{i \in A^+ \setminus S} \frac{\psi\left(|\omega_i|\right)}{\bar{\lambda}} x_i - \sum_{i \in A^- \setminus \overline{S}} \frac{\psi\left(|\omega_i|\right)}{\bar{\lambda}} x_i - \mathbf{x}(\overline{S}) \le |S| - \sum_{i \in A^- \setminus \overline{S}} \frac{\psi\left(|\omega_i|\right)}{\bar{\lambda}} - 1 \qquad (3.50)$$

where

$$\psi(a) = \begin{cases} h\bar{\lambda} & \textit{if } L_h \le a \le L_{h+1} - \bar{\lambda} \\ h\bar{\lambda} + (a - L_h) & \textit{if } L_h - \bar{\lambda} \le a \le L_h \\ p\bar{\lambda} + (a - L_p) & \textit{if } L_p - \bar{\lambda} \le a \end{cases},$$

is a superadditive lower bound on the lifting function of (3.48), $\bar{\lambda} := \sum_{j \in (S \cup A^- \setminus \bar{S})} |\omega_j| - b$ *and* $p = \left|\left\{i \in (S \cup \bar{S}) \ : \ |\omega_i| > \bar{\lambda}\right\}\right|$ *is valid for* $\mathrm{conv}(K_f)$.

3.5 Separating Submodular Cover Inequalities

In this section, we provide an algorithm to separate the submodular cover inequalities 3.41 for the submodular knapsack set K_f defined with respect to any submodular set function f.

Given a solution $\bar{\mathbf{x}}$ on the continuous relaxation of K_f, we wish to derive a valid submodular cover inequality that separates $\bar{\mathbf{x}}$ from $\mathrm{conv}\, K_f$. In particular, given $\bar{\mathbf{x}} \in \mathbb{R}^N$ such that $\mathbf{0} \le \bar{\mathbf{x}} \le \mathbf{1}$, we are interested in finding a submodular cover S with $\sum_{i \in S} \bar{x}_i - \sum_{i \in \bar{S}} \overline{x_i} > |S| - 1$, if there exists any.

As a preliminary, consider the set $\overline{I^+} = \{i \in N \ : \ \rho_i(N \setminus i) < 0\}$. It is easy to see that for any submodular cover S, $\bar{S} = \overline{I^+} \setminus S$. The separation problem with respect to the submodular cover inequalities can now be formulated as

$$\zeta = \max \left\{ \sum_{i \in N} (1 - \overline{x_i}) z_i + \sum_{i \in \overline{I^+}} \overline{x_i}(1 - z_i) \ : \ f(\mathbf{z}) > b, \ \mathbf{z} \in \{0,1\}^n \right\}, \tag{3.51}$$

where the constraint $f(\mathbf{z})$ ensures that $S_{\mathbf{z}}$ is a submodular cover. Observe that submodular cover corresponding to $\mathbf{z}$ yields a violated submodular cover inequality if and only if $\zeta < 1$.

Finding exact solutions to (3.51) is in general computationally expensive. The problem becomes further complicated when the closure of the continuous relaxation of feasible set corresponding to (3.51), namely the set $\{\mathbf{z} \in [0,1]^n \ : \ f(\mathbf{z}) \ge b\}$, is non-convex. Observe that any feasible solution $\bar{\mathbf{z}}$ to (3.51) satisfying $\zeta(\bar{\mathbf{z}}) = \sum_{i \in N} (1 - \overline{x_i}) \bar{z}_i + \sum_{i \in \overline{I^+}} \overline{x_i}(1 - \bar{z}_i) < 1$ yields a violated submodular cover inequality. In the following we provide an algorithm to yield a submodular cover S, if one exists.

Without loss of generality, assume that $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)^\top$ such that

$$\bar{x}_1 \ge \bar{x}_2 \ge \ldots \ge \bar{x}_n.$$

Algorithm 1 Greedy Algorithm to find Submodular Covers

procedure `GREEDY-SEP(`$\bar{\mathbf{x}}$`)`
  initialize $S = \emptyset$, $i = 1$
  while $f(S) \leq b$ **and** $i \leq n$ **do**
    if $\rho_i(S) > 0$ **and** $\rho_k(S \cup i \setminus k) > 0, \forall\, k \in S$ **then**
      update $z_i \leftarrow 1$, $S \leftarrow (S \cup i)$, $i \leftarrow (i+1)$
    else
      update $z_i \leftarrow 0$, $i \leftarrow (i+1)$
    end if
  end while
  return $\mathbf{z}$ and $S_{\mathbf{z}} = S$
end procedure

Proposition 3.47. *Let* $S =$ `GREEDY-SEP(`$\bar{\mathbf{x}}$`)`*, then exactly one of the following holds:*

(a) S *is a submodular cover.*

(b) $f(S \cup T) \leq b$ *for all* $T \subseteq N \setminus S$.

Proof. For $S =$ `GREEDY-SEP(`$\bar{\mathbf{x}}$`)` assume $f(S \cup T) \leq b$ for all $T \subseteq N \setminus S$. This implies, for $T = \emptyset$, $f(S) \leq b$. Hence S is not a submodular cover.

Alternatively, assume $S =$ `GREEDY-SEP(`$\bar{\mathbf{x}}$`)` is not a submodular cover. Since $\rho_k(S \setminus k) > 0$ for all $k \in S$, it must hold that $f(S) \leq b$. It suffices to show that $\nexists\, T \subseteq N \setminus S$ such that

(i) $f(S \cup T) > b$ and

(ii) $\rho_i(S \cup T \setminus i) > 0$ for all $i \in S \cup T$.

It follows from submodularity of f that (i) and (ii) hold *only if*

$$\rho_i(S) > 0 \text{ and } \rho_k(S \cup i \setminus k) > 0\, \forall\, k \in S, \text{ for all } i \in T.$$

Furthermore, observe that for all $i \in N \setminus S$, either $\rho_i(S) \leq 0$ or $\rho_k(S \cup i \setminus k) \leq 0$ for some $k \in S$.

The result follows. □

The submodular cover $S =$ `GREEDY-SEP(`$\bar{\mathbf{x}}$`)` yields a violated submodular cover inequality to separate a given $\bar{\mathbf{x}} \notin \text{conv}(K_f)$ if and only if $\zeta(\mathbf{z}_S) < 1$.

3.6 Computational Analysis

In this section we report our computational results with the submodular cover inequalities and their extensions. We tested the effectiveness of these inequalities on two different problems sets with and without structure. The first set of problems consist of randomly generated $0-1$ quadratically constrained problems with non-positive coefficients corresponding to all bilinear terms so that the resulting constraint is a general submodular knapsack. The second set also consists of $0-1$ quadratically constrained problems however without any assumptions on the coefficients.

All experiments were performed on a 2.93GHz Pentium Linux workstation with 8GB main memory using CPLEX* (version 12.6). We used CPLEX's barrier algorithm to solve quadratically constrained problems at the nodes of a branch-and-bound algorithm. CPLEX heuristics are turned off and a single thread is used. The search strategy is set to traditional branch-and-bound, rather than the default dynamic search as it is not possible to add user cuts in CPLEX while retaining the dynamic search strategy. CPLEX user cuts are turned off. In addition, the solver time limit and memory limit have been set to 3600 secs. and 4GB respectively for both sets of problem instances.

For both sets of problem instances we compare the performance of CPLEX with barrier algorithm, CPLEX with outer approximation, linearization via. extended polymatroid inequalities, and lifted covers derived via aggregated extended polymatroid inequalities. For the aggregation of the polymatroid inequalities we employ the following heuristic: we add the coefficients of all tight extended polymatroid inequalities and derive lifted covers using superadditive lifting technique. The cuts are added throughout the branch and bound tree. In all of the tabulated results we compare the algorithms with respect to following performance measures.

1. Integrality gap (igap).
2. Root relaxation gap (rgap).
3. End gap (egap).
4. Time to optimality in seconds (time).
5. Nodes explored in the branch-and-bound tree (nodes).
6. Number of instances solved to optimality (#).

Integrality gap (*igap*) is computed as $\dfrac{(f_u - f_i)}{f_u}$, where f_i denotes the objective value of the initial continuous relaxation and f_u denotes the objective of the best feasible solution found

*CPLEX is a registered trademark of IBM ILOG across all versions. The root gap (*rgap*) and the end gap (*egap*) are computed as $\dfrac{(f_u - f_r)}{f_u}$ and $\dfrac{(f_u - f_l)}{f_u}$, where f_r is the objective value of the relaxation at the root node and f_l is the best lower bound for the optimal objective at termination.

3.6.1 Submodular Quadratic Set Functions

Proposition 3.1 provides a characterization for a quadratic set function to be submodular. In particular, the problem set instances considered here are $0-1$ quadratically constrained knapsacks of the form

$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top \mathbf{x} \leq \gamma,\;\; Q_{ij} \leq 0,\;\; 1 \leq\, i,\, j\, \leq n\,,\, i \neq j.$$

In Tables 3.1 and 3.2 we report the results of the experiments for varying number of variables (n), and the number of constraints (m). For each combination, five random instances are generated where the coefficients for $\mathbf{Q}$ are generated from uniform $[-20, 0]$. Coefficients for $\mathbf{p}$ are generated from uniform $[0, 20]$. The knapsack budget γ is set to $0.5 * f(N)$. So that constraints are not completely dense, we set the density of the constraints to 50%.

For each solution procedure we report root relaxation gap, end gap, time to optimality, number of user cuts added, number of nodes explored in the branch-and-bound tree and the number of (out of five) instances solved to optimality. Each row in Tables 3.1 and 3.2 shows the averages of 5 instances.

In Table 3.1 we report the computational summary when the problem instances are solved using CPLEX barrier algorithm and CPLEX Outer Approximation strategy. As expected the root relaxation gaps and the number of nodes are higher for the outer approximation algorithm. Also observe that CPLEX cannot solve any of the problem instances in the given time limit for $n = 40$ and $m > 10$.

In Table 3.2 we present similar comparisons, but this time using the linearizations via extended polymatroid inequalities and lifted cover inequalities derived from aggregation of extended polymatroids. We report the number of respective cuts added in addition to the computational measures used earlier in Table 3.1. The high rgap values can be attributed to the fact that the extended polymatroids are linear relaxations of the original non-linear set. However the computational efficiency of these linearizations is evident from over 86.5% reduction in the solution times and the number of instances solved to optimality. When used in conjunction with the lifted covers obtained via aggregation of extended polymatroid inequalities the effectiveness of these linearization is further established. The root relaxation gaps are reduced by more than 42% on average. For the instances that are not solved to optimality within the time limit we see a reduction of 68% in the end gap values.

Table 3.1: Submodular QCP : Cplex barrier and cplex outer approximation

n	m	igap	CPLEX Barrier					CPLEX OA				
			rgap	egap	nodes	time	#	rgap	egap	nodes	time	#
30	1	23.8	23.8	0	697	1	5	25.3	0	6641	2	5
	5	23.5	23.5	0	6251	72	5	23.9	0	89036	184	5
	10	27.6	27.6	0	19035	620	5	27.7	0	139835	720	5
	20	28.7	28.7	0	9914	966	5	28.8	0	99122	519	5
	30	31	31	0.3	14674	2316	4	31.1	1	105185	1145	4
40	1	22.3	22.3	0	11648	28	5	25.3	1.9	148346	1030	4
	5	23.4	23.4	0	64183	1256	5	24.1	9.1	454805	3067	1
	10	24.4	24.4	3.1	51149	3092	1	24.8	15.7	386499	3588	0
	20	26.8	26.8	8.5	19228	3589	0	26.9	16	301495	3588	0
	30	27.9	27.9	12.6	11337	3589	0	28	21.9	152771	3588	0
Mean		**25.9**	**25.9**	**2.5**	**20812**	**1553**		**26.6**	**6.6**	**188374**	**1743**	
Stdev.		**2.9**	**2.9**					**2.3**				

Table 3.2: Submodular QCP : Extended polymatroids vs aggregated polymatroid covers

n	m	igap	Extended Polymatroids						Aggregated Polymatroid Covers						
			rgap	egap	cuts	nodes	time	#	rgap	egap	ep cuts	ac cuts	nodes	time	#
30	1	23.8	70	0	96	1579	0	5	10.8	0	443	53	50	0	5
	5	23.5	66.5	0	359	14036	4	5	10.5	0	343	1362	7995	20	5
	10	27.6	61.6	0	826	38913	21	5	19.1	0	803	4149	20748	66	5
	20	28.7	65.9	0	1077	30449	21	5	20	0	794	2656	14956	37	5
	30	31	64.3	0	1879	34357	42	5	24.1	0	1546	4404	21825	101	5
40	1	22.3	68.4	0	555	31293	16	5	10.1	0	1199	256	1504	5	5
	5	23.4	68	0	1207	155869	221	5	9	0	915	4694	41969	417	5
	10	24.4	63	1.7	1685	291989	397	4	12.7	1.3	1259	642669	80785	1075	3
	20	26.8	67.4	1.9	3196	266027	809	4	14.8	0.9	1446	8303	102717	934	4
	30	27.9	60.4	9.1	4686	152921	547	1	20.9	6.2	2893	573563	80939	1269	1
Mean		**25.9**	**65.6**	**1.3**	**1557**	**101743**	**208**		**15.2**	**0.8**	**1164**	**124211**	**37349**	**392**	
Stdev.		**2.9**	**3.1**						**5.4**						

3.6.2 General Quadratic Set Functions

The second set of problem instances belong to the general quadratic set functions. We relax the restrictions on the matrix $\mathbf{Q}$ as imposed in previous set of problem data. In particular, we solve general $0-1$ quadratically constrained problems. The constraint set in context is

$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top \mathbf{x} \leq \gamma.$$

Since the set function in context is not necessarily submodular, the inequalities derived in this paper cannot be applied to the problem instances as is. We reformulate the set function $f(\mathbf{x})$ using additional variables $\mathbf{z}$ to yield a submodular set function $f(\mathbf{x}, \mathbf{z})$.

For all the bilinear terms in the quadratic function with positive coefficients we can relax the bilinearity using McCormick Relaxations [66]. Specifically, we define $z_{ij} = x_i x_j$ s.t.

$$\begin{aligned} z_{ij} &\geq (x_i + x_j - 1)^+ \\ z_{ij} &\leq \min(x_i, x_j), \end{aligned}$$

for all pairs $(ij)\ :\ Q_{ij} > 0$. The set function $f(\mathbf{x}, \mathbf{z})$ thus obtained

$$f(\mathbf{x}, \mathbf{z}) = \sum_i Q_{ii} x_i + \sum_{ij:Q_{ij} \leq 0} Q_{ij} x_i x_j + \sum_{ij:Q_{ij}>0} Q_{ij} z_{ij} + \mathbf{p}^\top \mathbf{x} \leq \gamma$$

is submodular.

Table 3.3: General $0-1$ QCP : Cplex barrier and cplex outer approximation

n	m	igap	CPLEX Barrier					CPLEX OA				
			rgap	egap	nodes	time	#	rgap	egap	nodes	time	#
30	10	59.06	59.06	0	4046	136.9	5	59.17	0	38993	80.9	5
	20	64.45	64.45	0	1532	162.8	5	64.7	0	28252	89.6	5
	30	54.88	54.88	0	3403	665.4	5	54.93	0	55069	382.3	5
40	10	72.16	72.16	0	1069	56.2	5	72.31	0	15889	27.3	5
	20	61.38	61.38	0	5426	1204.9	5	61.9	3.42	102359	888.2	4
	30	57.2	57.2	12.78	5367	2446.9	2	57.56	18.37	137770	2575.7	2
50	10	65.3	65.3	5.35	8686	907.5	4	65.75	9.61	114396	1224.4	4
	20	63.97	63.97	15.25	6379	2419.4	3	64.54	22.66	129926	2078.1	3
	30	58.92	58.92	26.36	3466	2961.6	1	59.42	32.91	151610	2872.3	1
Mean		**61.9**	**61.9**	**6.6**	**4375**	**1218**		**62.3**	**9.7**	**86029**	**1135**	
Stdev.		**5.2**	**5.2**					**5.2**				

In Tables 3.3 and 3.4 we report the results of the experiments for varying number of variables (n), and the number of constraints (m). For each combination, five random instances are generated where the coefficients for $\mathbf{Q}, \mathbf{p}$ are generated from uniform $[-20, 20]$. The knapsack budget γ is set to $0.5 * f(N)$. So that constraints are not completely dense, we set the density of the constraints to 50%.

For each solution procedure we report root relaxation gap, end gap, time to optimality, number of user cuts added, number of nodes explored in the branch-and-bound tree and the number of (out of five) instances solved to optimality. Each row in Tables 3.3 and 3.4 shows the averages of 5 instances.

Table 3.4: General $0-1$ QCP : Extended polymatroids vs aggregated polymatroid covers

n	m	igap	Extended Polymatroids						Aggregated Polymatroid Covers						
			rgap	**egap**	**cuts**	**nodes**	**time**	**#**	**rgap**	**egap**	**ep cuts**	**ac cuts**	**nodes**	**time**	**#**
30	10	59.06	91	0	471	9337	11.4	5	51.73	0	1703	34	2148	10.6	5
	20	64.45	93.31	0	382	4550	5.2	5	50.96	0	1064	45	1381	4.3	5
	30	54.88	86.1	0	808	13131	44	5	43.56	0	1557	47	7361	30.9	5
40	10	72.16	91.63	0	298	2917	2.7	5	50.22	0	1698	13	105	7.4	5
	20	61.38	90.01	0	853	37927	287.3	5	40.79	0	4013	41	11415	215.4	5
	30	57.2	89.24	1.34	2867	94947	1544.4	4	45.14	0	5306	220	53934	1275.8	5
50	10	65.3	91.94	6.45	1293	42550	747.6	4	36.08	4.9	5464	22	5318	745.1	4
	20	63.97	95.58	8.08	3215	63312	1448	4	46.31	5.61	4734	145	21624	1084.3	4
	30	58.92	89.3	17.61	5192	91698	2870.2	1	49.32	12.7	8479	186	35091	2290.8	2
Mean		**61.9**	**90.9**	**3.7**	**1709**	**40041**	**773**		**46**	**3**	**3780**	**84**	**15375**	**629**	
Stdev.		**5.2**	**2.7**						**5.2**						

As in the previous case, in Table 3.3 we report the computational summary when the problem instances are solved using CPLEX barrier algorithm and CPLEX Outer Approximation strategy. In Table 3.4 we present similar comparisons, but this time using the linearizations via extended polymatroid inequalities and lifted cover inequalities derived from aggregation of extended polymatroids. Similar to our observations in the case of submodular quadratically constrained problem sets we see that application of extended polymatroid inequalities improved the solution times reduce by over 36.5%. Using aggregated polymatroid covers on these problem instances furthers this observation. We see a root gap reduction of 25% when using these inequalities that translates into halving the solution times on average for the problem instances in this case.

Chapter 4

Convex Envelopes of Binary Quadratic Sets

4.1 Introduction

In Chapter 3 we studied the submodular knapsack polytope and derived valid inequalities for the same. We also provided a reformulation for a general quadratic knapsack to a submodular quadratic knapsack. Taking a detour from the combinatorial discussion of the $0-1$ conic-quadratic sets, this chapter provides a slightly different geometrical perspective. In this chapter we provide a brief discussion for some convexification techniques for $0-1$ non-convex quadratic sets. We will also establish some geometrical understanding with respect to these convexifications. In addition, a key result of this chapter yields a recipe to half the number of constraints used in standard linearization of the $0-1$ quadratic sets in a higher dimensional space.

4.2 The Sums of Squares (SOS) Reformulation

For $t_0 \in \mathbb{R}$ define

$$F := \left\{(x,y) \in [0,1]^2 \ : \ \pm xy \leq t_0\right\} \tag{4.1}$$

$$\overline{F} := \left\{(x,y) \in [0,1]^2 \ : \ (x \pm y)^2 \leq x + y + 2t_0\right\} \tag{4.2}$$

While F is not necessarily convex, $\overline{F}$ is convex. In addition

1. $F \subseteq \overline{F}$,
2. $F \cap \mathbb{Z}^2 = \overline{F} \cap \mathbb{Z}^2$.

This provides us with a means to derive convex reformulations of the general binary knapsack sets. Consider the following.

Definition 4.1. Let $\mathbf{Q} = [\, q_{ij} \,]_{1 \le i,j \le n} \in \mathbb{R}^{n \times n}$ be any real $n \times n$ matrix map, $\mathbf{p} = [\, p_i \,]_{1 \le i \le n} \in \mathbb{R}^n$ be any n dimensional real vector and $r \in \mathbb{R}$ be a constant. We define F and $\tilde{F}$ as

$$F := \left\{ \mathbf{x} \in [0,1]^n \; : \; \mathbf{x}^\top \mathbf{Q}\, \mathbf{x} + \mathbf{p}^\top \mathbf{x} + r \ge 0 \right\} \tag{4.3}$$

$$\begin{aligned} \tilde{F} := \Bigg\{ \mathbf{x} \in [0,1]^n \; : \; & \sum_{i=1}^{n} \sum_{j=1}^{n} \left[q_{ij}^{+} \frac{(x_i - x_j)^2}{2} + q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right] \\ & \le \sum_{i=1}^{n} \sum_{j=1}^{n} |q_{ij}| \left(\frac{x_i + x_j}{2} \right) + \mathbf{p}^\top \mathbf{x} + r \Bigg\} \end{aligned} \tag{4.4}$$

Proposition 4.1. *Let F and $\tilde{F}$ be defined as in 4.3 and 4.4 respectively, then*

(i) $F \subseteq \tilde{F}$,

(ii) $F \cap \mathbb{Z}^n = \tilde{F} \cap \mathbb{Z}^n$.

Proof. Consider $\mathbf{x} \in F$. We have

$$\begin{aligned} \mathbf{x}^\top \mathbf{Q}\, \mathbf{x} + \mathbf{p}^\top \mathbf{x} + r &\ge 0 \\ \mathbf{p}^\top \mathbf{x} + r &\ge -\mathbf{x}^\top \mathbf{Q}\, \mathbf{x} \\ &= -\sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} x_i x_j \\ &= -\sum_{i=1}^{n} \sum_{j=1}^{n} \left[q_{ij}^{+} x_i x_j - q_{ij}^{-} x_i x_j \right] \\ &\ge -\sum_{i=1}^{n} \sum_{j=1}^{n} \left[q_{ij}^{+} x_i x_j - q_{ij}^{-} x_i x_j + (q_{ij}^{+} + q_{ij}^{-}) \frac{(x_i - x_i^2 + x_j - x_j^2)}{2} \right] \\ &= -\sum_{i=1}^{n} \sum_{j=1}^{n} \left[(q_{ij}^{+} + q_{ij}^{-}) \left(\frac{x_i + x_j}{2} \right) - q_{ij}^{+} \frac{(x_i - x_j)^2}{2} - q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right] \end{aligned}$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} (q_{ij}^{+} + q_{ij}^{-}) \left(\frac{x_i + x_j}{2} \right) + \mathbf{p}^\top \mathbf{x} + r \ge \sum_{i=1}^{n} \sum_{j=1}^{n} \left[q_{ij}^{+} \frac{(x_i - x_j)^2}{2} + q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right]$$

$$\Rightarrow \qquad \mathbf{x} \in \tilde{F}.$$

Third inequality above follows from the fact that $x^2 \le x, \; x \in [0,1]$ where equality holds *iff* $x \in \{0,1\}$. □

Proposition 4.1 yields convex relaxations for the non-convex set F.

Definition 4.2. Define the set of indices

$$I := \left\{ i \;:\; q_{ii} + p_i + \sum_{j=1}^{n} (q_{ij}^{+} + q_{ji}^{+}) + |r| < 0,\; 1 \le i \le n \right\}.$$

Definition 4.3. Define the set

$$F^c := \left\{ \mathbf{x} \in \{0,1\}n \;:\; \sum_{i \in I} x_i \ge 1,\; x_j = 0,\; \forall\, j \in N \setminus I \right\}.$$

Proposition 4.2. *$F \cap F^c = \emptyset$.*

Proof. Assume $\exists\, \mathbf{x} \in F \cap F^c$ such that $\sum_{i \in I} x_i = k \ge 1$. Then

$$\begin{aligned}
0 \le\; & \mathbf{x}^\top \mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top \mathbf{x} + r \\
= & \sum_{i=1}^{n} \left(q_{ii} + p_i + \sum_{\substack{j=1 \\ j \ne i}}^{n} (q_{ij}^{+} + q_{ji}^{+}) x_i - \sum_{\substack{j=1 \\ j \ne i}}^{n} (q_{ij}^{-} + q_{ji}^{-}) x_j \right) x_i + r \\
= & \sum_{i \in I} \left(q_{ii} + p_i + \sum_{\substack{j \in I \\ j \ne i}} (q_{ij}^{+} + q_{ji}^{+}) x_j \right) - \sum_{\substack{j \in I \\ j \ne i}} (q_{ij}^{-} + q_{ji}^{-}) x_i x_j + r \\
< & -k|r| + r - \sum_{\substack{j \in I \\ j \ne i}} (q_{ij}^{-} + q_{ji}^{-}) x_i x_j.
\end{aligned}$$

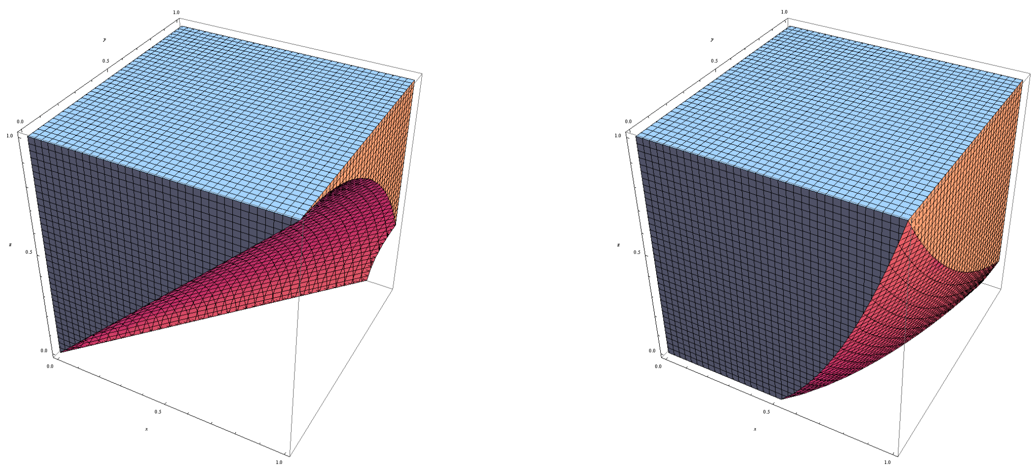
However this presents a contradiction since $-\sum_{\substack{j \in I \\ j \ne i}} (q_{ij}^{-} + q_{ji}^{-}) x_i x_j \le 0$ and $k \ge 1$ implies $-k|r| + r \le 0$. □

Example 4.1. Consider the sets

$$\begin{aligned}
F &= \left\{ (x,y,z) \in [0,1]^3 \;:\; x^2 \le y^2 + z^2 - 0.2xy + 0.27yz \right\}, \\
\tilde{F} &= \left\{ (x,y,z) \in [0,1]^3 \;:\; 0.135(y-z)^2 + 0.1(x+y)^2 + 2x^2 \le 1.1x + 1.235y + 1.135z \right\}.
\end{aligned}$$

Figures 4.1(a) and 4.1(b) represent the non-convex set F and convex relaxation $\tilde{F}$.

Observe that $F \cap \mathbb{Z}^n = \tilde{F} \cap \mathbb{Z}^n = \{(0,0,0), (0,0,1), (0,1,0), (0,1,1), (1,0,1), (1,1,1)\}$. In addition, we have $I = \{1\}$ and $F^c = \{(1,0,0)\}$. Clearly $F \cap F^c = \emptyset$.



(a) Non-convex set F (b) convex relaxation $\tilde{F}$

Figure 4.1: Non-convex set F and the convex relaxation $\tilde{F}$

4.3 Strengthening the SOS Relaxation

Definition 4.4. Define the set $\overline{F}$ as

$$\overline{F} := \left\{ \mathbf{x} \in [0,1]^n : \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} \left(q_{ij}^{+} \frac{(x_i - x_j)^2}{2} + q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right) + q_{ii}^{-} x_i^2 \right] \right.$$
$$\left. \leq \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} |q_{ij}| \left(\frac{x_i + x_j}{2} \right) + q_{ii}^{+} x_i \right] + \mathbf{p}^{\top}\mathbf{x} + r \right\}. \tag{4.5}$$

Proposition 4.3. *For F, $\tilde{F}$ and $\overline{F}$ defined as in 4.3, 4.4 and 4.5 respectively,* $\overline{F} \subseteq \tilde{F}$.

Proof. (*i*) $F \subseteq \overline{F}$

Consider $\mathbf{x} \in F$. Now

$$\begin{aligned}
\mathbf{x}^\top \mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top \mathbf{x} + r &\geq 0 \\
\mathbf{p}^\top \mathbf{x} + r &\geq -\mathbf{x}^\top \mathbf{Q}\,\mathbf{x} \\
&= -\sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} x_i x_j \\
&= -\sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \left[q_{ij}^{+} x_i x_j - q_{ij}^{-} x_i x_j \right] + \sum_{i=1}^{n} q_{ii}^{-} x_i^2 - \sum_{i=1}^{n} q_{ii}^{+} x_i^2
\end{aligned}$$

$$\begin{aligned}
\mathbf{p}^\top \mathbf{x} + r &\geq -\sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \left[q_{ij}^{+} x_i x_j - q_{ij}^{-} x_i x_j + |q_{ij}| \frac{(x_i - x_i^2 + x_j - x_j^2)}{2} \right] + \sum_{i=1}^{n} q_{ii}^{-} x_i^2 - \sum_{i=1}^{n} q_{ii}^{+} x_i \\
&= -\sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \left[|q_{ij}| \left(\frac{x_i + x_j}{2} \right) - q_{ij}^{+} \frac{(x_i - x_j)^2}{2} - q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right] + \sum_{i=1}^{n} q_{ii}^{-} x_i^2 - \sum_{i=1}^{n} q_{ii}^{+} x_i
\end{aligned}$$

$$\sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} |q_{ij}| \left(\frac{x_i + x_j}{2} \right) + q_{ii}^{+} x_i \right] + \mathbf{p}^\top \mathbf{x} + r$$

$$\geq \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} \left(q_{ij}^{+} \frac{(x_i - x_j)^2}{2} + q_{ij}^{-} \frac{(x_i + x_j)^2}{2} \right) + q_{ii}^{-} x_i^2 \right].$$

$\Rightarrow \mathbf{x} \in \overline{F}$.
Third inequality follows from the fact that $x^2 \leq x,\ x \in [0,1]$.
(ii) $\overline{F} \subseteq \tilde{F}$

Consider $\mathbf{x} \in \overline{F}$. We have

$$\sum_{i=1}^{n}\left[\sum_{\substack{j=1\\j\neq i}}^{n}|q_{ij}|\left(\frac{x_i+x_j}{2}\right)+q_{ii}^{+}x_i\right]+\mathbf{p}^\top\mathbf{x}+r$$

$$\geq \sum_{i=1}^{n}\left[\sum_{\substack{j=1\\j\neq i}}^{n}\left(q_{ij}^{+}\frac{(x_i-x_j)^2}{2}+q_{ij}^{-}\frac{(x_i+x_j)^2}{2}\right)+q_{ii}^{-}x_i^2\right]$$

$$\geq \sum_{i=1}^{n}\left[\sum_{\substack{j=1\\j\neq i}}^{n}\left(q_{ij}^{+}\frac{(x_i-x_j)^2}{2}+q_{ij}^{-}\frac{(x_i+x_j)^2}{2}\right)+q_{ii}^{-}x_i^2+q_{ii}^{-}(x_i^2-x_i)\right]$$

$$\sum_{i=1}^{n}\left[\sum_{\substack{j=1\\j\neq i}}^{n}|q_{ij}|\left(\frac{x_i+x_j}{2}\right)+|q_{ii}|x_i\right]+\mathbf{p}^\top\mathbf{x}+r \geq$$

$$\sum_{i=1}^{n}\left[\sum_{\substack{j=1\\j\neq i}}^{n}\left(q_{ij}^{+}\frac{(x_i-x_j)^2}{2}+q_{ij}^{-}\frac{(x_i+x_j)^2}{2}\right)+q_{ii}^{-}\frac{(x_i+x_i)^2}{2}\right]$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}|q_{ij}|\left(\frac{x_i+x_j}{2}\right)+\mathbf{p}^\top\mathbf{x}+r \geq \sum_{i=1}^{n}\sum_{j=1}^{n}\left[q_{ij}^{+}\frac{(x_i-x_j)^2}{2}+q_{ij}^{-}\frac{(x_i+x_j)^2}{2}\right]$$

$$\Rightarrow \qquad \mathbf{x} \in \tilde{F}.$$

Second inequality follows from the fact that $x^2 \leq x,\ x \in [0,1]$. □

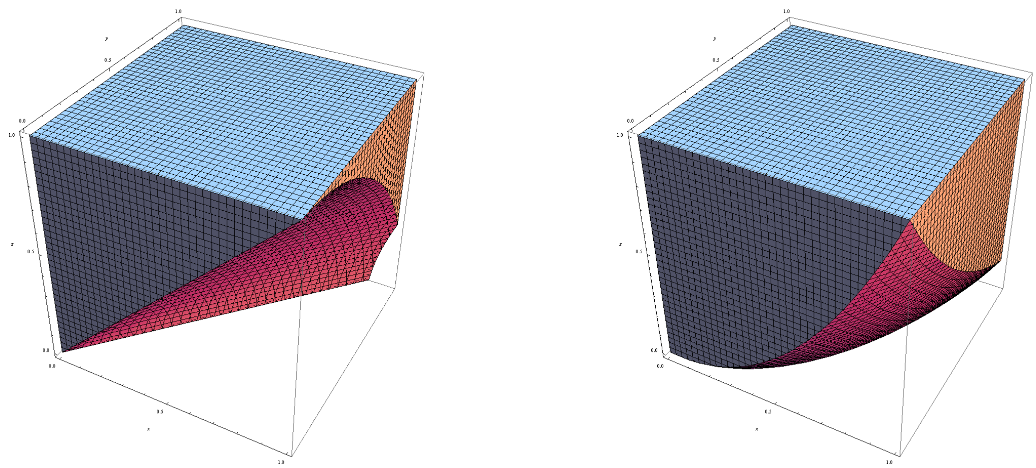
Corollary 4.1. $F \cap \mathbb{Z}^n = \overline{F} \cap \mathbb{Z}^n = \tilde{F} \cap \mathbb{Z}^n$.

Example 4.2. Consider the sets as defined in Example 4.1

$$F = \left\{(x,y,z) \in [0,1]^3 \ :\ x^2 \leq y^2+z^2-0.2xy+0.27yz\right\}$$
$$\tilde{F} = \left\{(x,y,z) \in [0,1]^3 \ :\ 0.135(y-z)^2+0.1(x+y)^2+2x^2 \leq 1.1x+1.235y+1.135z\right\}$$

A stronger convex relaxation for F is given by

$$\overline{F} = \left\{(x,y,z) \in [0,1]^3 \ :\ 0.135(y-z)^2+0.1(x+y)^2+x^2 \leq 0.1x+1.235y+1.135z\right\}$$



(a) Non-convex set F (b) convex relaxation $\overline{F}$

Figure 4.2: Non-convex set F and the convex relaxation $\overline{F}$

Figure 4.2(b) represents the convex relaxation $\overline{F}$

In addition observe the face $y = 1$ in the following for the two relaxations as compared to F.

Definition 4.5. Define the set of indices J and the set $X \subseteq F$ as

$$\begin{aligned} J &:= \left\{ j \in \{1, 2, \ldots, n\} \ : \ q^+_{jj} > 0 \right\}, \\ X &:= \left\{ \mathbf{x} \in [0,1]^n \ : \ x_j \in \{0,1\} \ \ \forall\, j \in J \right\}. \end{aligned}$$

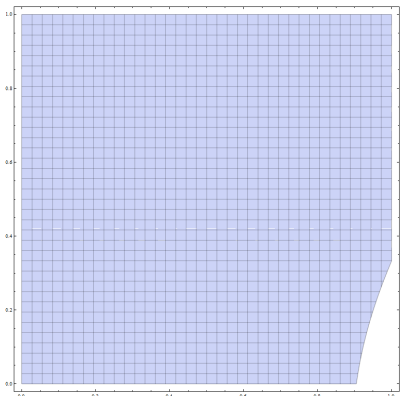
Proposition 4.4. *If* $q_{ij} = 0 \ \forall\ i \in N \setminus J,\ j \in N, j \neq i$, *then,* $\overline{F} \cap X = F \cap X$.

Proof. Assume, $q_{ij} = 0 \ \forall\ i \in N \setminus J,\ j \in N, j \neq i$. It follows from Proposition 4.3 that $\overline{F} \cap X \supseteq F \cap X$. Thus it suffices to show that $\overline{F} \cap X \subseteq F \cap X$.

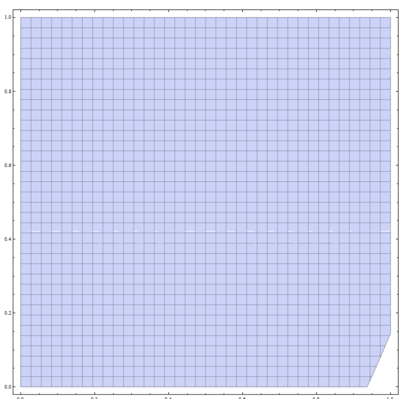
Consider $\mathbf{x} \in \overline{F} \cap X$. We have

$$\sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} |q_{ij}| \left(\frac{x_i + x_j}{2} \right) + q^+_{ii} x_i \right] + \mathbf{p}^\top \mathbf{x} + r$$

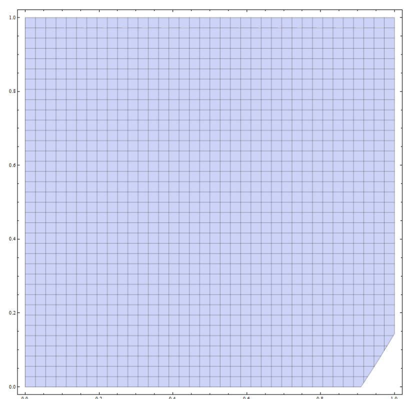
$$\geq \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} \left(q^+_{ij} \frac{(x_i - x_j)^2}{2} + q^-_{ij} \frac{(x_i + x_j)^2}{2} \right) + q^-_{ii} x_i^2 \right]$$



(a) F



(b) $\tilde{F}$



(c) $\overline{F}$

Figure 4.3: Non-convex set F and the convex relaxations $\tilde{F}$ and $\overline{F}$, face $y = 1$

$$\sum_{i=1}^{n}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}|q_{ij}|\left(\frac{x_i + x_j}{2}\right) + q_{ii}^{+}x_i^2 - q_{ii}^{-}x_i^2\right] + \mathbf{p}^{\top}\mathbf{x} + r$$

$$\geq \sum_{i=1}^{n}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}\left(q_{ij}^{+}\frac{(x_i - x_j)^2}{2} + q_{ij}^{-}\frac{(x_i + x_j)^2}{2}\right)\right]$$

$$
\begin{aligned}
\sum_{i=1}^{n}\sum_{j=1}^{n} q_{ij}x_ix_j + \mathbf{p}^\top\mathbf{x} + r &\geq \sum_{i\in N\setminus J}\ \sum_{j\in N\setminus J} |q_{ij}| \left(\frac{(x_i - x_i^2 + x_j - x_j^2)}{2}\right)\\
&= 0\\
\Rightarrow \qquad\qquad\qquad\qquad & \mathbf{x} \in F\cap X.
\end{aligned}
$$

The last equality follows from the stated assumption. □

Proposition 4.4 yields strong convex relaxations with exact extreme points for the feasible sets of the form

$$
P := \left\{(\mathbf{x},\mathbf{y}) \in \{0,1\}n \times \mathbb{R}^m \ : \ \mathbf{y}^\top \tilde{\mathbf{Q}}\,\mathbf{y} + \tilde{\mathbf{p}}^\top\mathbf{y} \leq \mathbf{x}^\top\mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top\mathbf{x} + r\right\},
$$

where $\tilde{\mathbf{Q}} \in \mathbb{R}^{m\times m}_{\succeq 0}$ and $\tilde{\mathbf{p}} \in \mathbb{R}^m$. An intuition to this is that since the left hand side is already convex and Proposition 4.3 gives a means to convexify the right hand side.

Before we proceed further, observe the following preliminary. Let $\mathbf{Q}$ be a $n\times n$ matrix with real eigenvalues and a spectral decomposition $\mathbf{Q} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^\top$, then

1. $q_{ij} = \sum_{k=1}^{n} \lambda_k u_{ik}u_{jk}$,
2. $\mathbf{Q} \succeq 0 \Rightarrow q_{ii} \geq 0 \ \ \forall\ i \in \{1,2,\dots,n\}$.

4.4 A Convexification Approach *via* Eigendecomposition

Proposition 4.5. *Let $\mathbf{Q} \in \mathbb{R}^{n\times n}$ be a $n\times n$ matrix with real eigenvalues and a spectral decomposition as, $\mathbf{Q} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^\top$. Let F_Λ be defined as*

$$
\begin{aligned}
F_\Lambda := \Bigg\{ \mathbf{x}\in[0,1]^n : \sum_{i=1}^{n}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}\left(\hat{q}^+_{ij}\frac{(x_i-x_j)^2}{2} + \hat{q}^-_{ij}\frac{(x_i+x_j)^2}{2}\right) + \lambda_i^-(\mathbf{u}_i^\top\mathbf{x})^2\right]&\\
\leq \sum_{i=1}^{n}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}|\hat{q}_{ij}|\left(\frac{x_i+x_j}{2}\right) + \hat{q}_{ii}x_i\right] + \mathbf{p}^\top\mathbf{x} + r &\Bigg\},
\end{aligned}
$$

where $\hat{q}_{ij} = \displaystyle\sum_{k=1}^{n} \lambda_k^+ u_{ik}u_{jk} \ \ \forall\ i,j \in \{1,2,\dots,n\}$ and $\mathbf{u}_i$ denotes the i^{th} column of $\mathbf{U}$, then $F \subseteq F_\Lambda$.

Proof. Consider $\mathbf{x} \in F$, thus,

$$\begin{aligned}
\mathbf{x}^\top \mathbf{Q}\,\mathbf{x} + \mathbf{p}^\top \mathbf{x} + r &\geq 0 \\
\mathbf{p}^\top \mathbf{x} + r &\geq -\mathbf{x}^\top \mathbf{Q}\,\mathbf{x} \\
&= -\mathbf{x}^\top \mathbf{U}\,\boldsymbol{\Lambda}\,\mathbf{U}^\top \mathbf{x} \\
&= -\sum_{i=1}^{n} \lambda_i (\mathbf{u}_i^\top \mathbf{x})^2 \\
&= \sum_{i=1}^{n} \lambda_i^- (\mathbf{u}_i^\top \mathbf{x})^2 - \sum_{i=1}^{n} \lambda_i^+ (\mathbf{u}_i^\top \mathbf{x})^2 \\
&= \sum_{i=1}^{n} \lambda_i^- (\mathbf{u}_i^\top \mathbf{x})^2 - \sum_{i=1}^{n} \lambda_i^+ (\mathbf{u}_i^\top \mathbf{x})^2 \\
&= \sum_{i=1}^{n} \lambda_i^- (\mathbf{u}_i^\top \mathbf{x})^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} \hat{q}_{ij} x_i x_j \\
&\geq \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} \left(\hat{q}_{ij}^+ \frac{(x_i - x_j)^2}{2} + \hat{q}_{ij}^- \frac{(x_i + x_j)^2}{2} \right) + \lambda_i^- (\mathbf{u}_i^\top \mathbf{x})^2 \right] \\
&\qquad - \sum_{i=1}^{n} \left[\sum_{\substack{j=1 \\ j \neq i}}^{n} |\hat{q}_{ij}| \left(\frac{x_i + x_j}{2} \right) + \hat{q}_{ii} x_i \right]
\end{aligned}$$

The result follows. $\square$

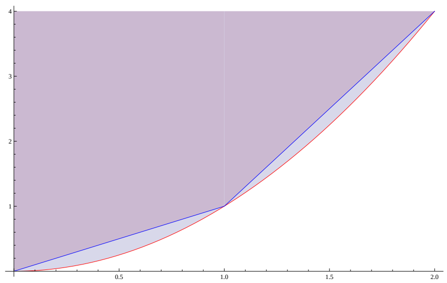
4.5 Strengthening SOS Relaxation *via* Linearization

For any $x_i, x_j \in \{0,1\}$ define

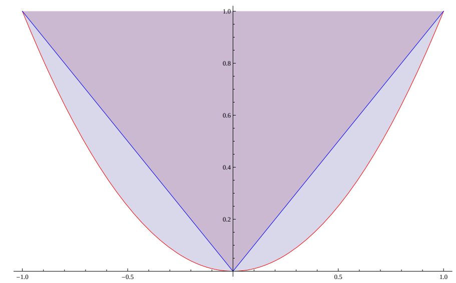
$$\begin{aligned}
\overline{F}_{ij}^+ &= \left\{ (x_i, x_j, y_{ij}) \in \{0,1\}^2 \times \mathbb{Z} \;:\; (x_i + x_j)^2 \leq y_{ij} \right\}, \\
P_{ij}^+ &= \left\{ (x_i, x_j, y_{ij}) \in [0,1]^2 \times \mathbb{R} \;:\; \max\{3(x_i + x_j) - 2, x_i + x_j\} \leq y_{ij} \right\}, \\
\overline{F}_{ij}^- &= \left\{ (x_i, x_j, y_{ij}) \in \{0,1\}^2 \times \mathbb{Z} \;:\; (x_i - x_j)^2 \leq y_{ij} \right\}, \\
P_{ij}^- &= \left\{ (x_i, x_j, y_{ij}) \in [0,1]^2 \times \mathbb{R} \;:\; |x_i - x_j| \leq y_{ij} \right\}.
\end{aligned}$$

It follows that

1. $P_{ij}^+ = \text{conv}(\overline{F}_{ij}^+)$,
2. $P_{ij}^- = \text{conv}(\overline{F}_{ij}^-)$.



(a) $t^2 \leq s,\ \max\{t, 3t-2\} \leq s,\ 0 \leq t \leq 4$



(b) $t^2 \leq s,\ |t| \leq s,\ 0 \leq t \leq 4$

Figure 4.4: Strengthening the SOS reformulation via linearization

The following result is immediate.

Proposition 4.6. *For set P defined as*

$$P := \{(\mathbf{x}, \mathbf{y}) \in \{0,1\}^n \times \mathbb{R}^{\binom{n}{2}} | \sum_{i=1}^{n} \left[\sum_{j>i}^{n} \left(q_{ij}^+ y_{ij}^- + q_{ij}^- y_{ij}^+ - |q_{ij}|(x_i + x_j) \right) - q_{ii} x_i \right] \leq 0$$
$$|x_i - x_j| \leq y_{ij}^- \quad \forall (i,j) : q_{ij} > 0$$
$$\max\{3(x_i + x_j) - 2, x_i + x_j\} \leq y_{ij}^+ \ \forall (i,j) : q_{ij} < 0\},$$

$\mathbf{Proj_y}\, P = F \cap \mathbb{Z}^n$.

Observe that the linearizations derived in Proposition 4.6 are a modified version of the McCormick linearizations with half the number of constraints. McCormick linearizations [66] linearize each bilinear term using four inequalities, however only two suffice for each bilinear term. SOS linearizations provide a way to distinguish these sufficient inequalities. The two sufficient inequalities depend only on the sign of the coefficient of the bilinear term.

Chapter 5

Network design with uncertain arc capacities

This chapter presents an application of the solution approaches discussed in this dissertation. We address the network design problem with uncertain arc capacities. We formulate the robust network design problem as a $0-1$ conic quadratic program without particular assumptions on the characteristics of uncertainties.

5.1 Introduction

Uncertainties in network design problems have been primarily addressed in the previous literature from the viewpoint of uncertain demands and costs [13, 25, 32, 79]. While these parameters are certainly important, another crucial issue that needs to be addressed in many real-world situations is the presence of potential disruptions of network arcs, which are uncertain by nature and may be caused by natural or artificial factors. In the context of transportation network infrastructure (e.g., air or ground transportation), the uncertain disruptions are often caused by weather conditions along with many other possible factors. Similar issues also often occur in the design and operation of communication network infrastructure, power grid, and related applications [53].

The main conceptual difference of the problem setup with multiple uncertain arc capacities from the previously considered problem formulations with uncertain demands and/or costs is the fact that the structure (topology) of the network itself is not deterministic anymore, which creates challenges in terms of optimal robust flow assignments in these networks, since the obtained optimal solutions need to be not only cost efficient, but also robust with respect to potential arc capacity disruptions. These disruptions can cause the reduced flow through a network, and the important question that needs to be rigorously addressed is: *How to efficiently minimize the costs of network design in the framework of large-scale fixed-charge network flow problems with probabilistic arc capacities?*

In this paper, we address both the conceptual and computational issues associated with the above question. Specifically, this paper addresses the network design problem with uncertainties in arc capacities. Using concepts from robust optimization, we formulate the robust network design problem as a $0-1$ conic quadratic program without particular assumptions on the characteristics of uncertainties. We propose a row generation approach to ascertain demand satisfaction at each possible s-t cut in the network, yielding an iterative solution procedure for the problem. We show that when capacities are independent, under mild assumptions, the feasible set is the intersection of supermodular covering knapsacks. A reformulation of the problem is proposed in the presence of correlations in order to recover the combinatorial structure of the set function in the underlying constraints. We show that exploring this combinatorial structure of problem significantly reduces the LP relaxation gaps and the solution times. The separation problem for the constraints is modeled as a robust minimum cut problem. We show that this separation problem is NP hard and provide reformulations to obtain computationally effective solution procedures. Finally, we present a computational analysis contrasting the various solution methodologies discussed in the paper to solve the problem to global optimality.

The remainder of this paper is organized as follows: In Section 5.2 we present a formulation for network design problem with uncertain capacities. Section 5.5 entails outlining the separation problem in the case of both uncorrelated and correlated capacities respectively. In Section 5.6 we present the computational results contrasting the efficiency of discussed solution approaches *vis-à-vis* CPLEX in case of both uncorrelated and correlated capacities.

5.1.1 Network Design with Uncertain Capacities

Consider a flow network $N(V, A)$, with n nodes, m arcs, a single source s and a single sink t. Observe that the assumption of single source and single sink can be made without loss of generality, since we can collate multiple sources and sinks into one node each respectively via arcs with deterministic capacities. The arc capacities ξ_{ij} in $N(V, A)$ are assumed to be random with a support Ξ. Every arc $(ij) \in A$ has a fixed, one time cost f_{ij} associated with it (the variable costs incurred as a part of per unit flow through the arcs have been assumed to be negligent in comparison with fixed costs and are ignored for the purpose of analysis). With the aforementioned setup, we illustrate the problem of determining the network setup with minimum cost that satisfies the demand with at least probability $1-\epsilon$, $(0 < \epsilon < 0.5)$. Since the capacities are stochastic, we need to ensure that every s-t cut in the network satisfies the demand probabilistically. We write the *demand satisfiability constraints* as

$$\mathbb{P}\left(\sum_{e \in C} \xi_e x_e \geq d\right) \geq 1-\epsilon \quad \forall\, C \in \mathcal{C}, \tag{5.1}$$

where $\mathbf{x} \in \{0,1\}^m$ denotes the arc assignments in a network setup and $\mathcal{C}$ denotes the set of all s-t cuts in the network $N(V, A)$.

Demand satisfiability constraints (5.1) thus ensure that any s-t cut in the feasible network setup will have a flow of at least d with a confidence level $1-\epsilon$. Notice that if $\boldsymbol{\xi}$'s are normally distributed independent random variables, then letting $\mathbf{u}$ and $\boldsymbol{\Sigma}$ denote the mean and variance covariance matrix of $\boldsymbol{\xi}$, the set of $0-1$ solutions satisfying (5.1) is exactly the following conic quadratic 0-1 covering knapsack

$$X := \left\{ \mathbf{x} \in \{0,1\}^m \ : \ \mathbf{u}^\top \mathbf{x} - \Omega \parallel \boldsymbol{\Sigma}^{1/2} \mathbf{x} \parallel \geq d \right\}, \tag{5.2}$$

where $\Omega = \varphi^{-1}(\epsilon)$, $(0 \leq \epsilon \leq 0.5)$ and φ is the standard normal cumulative distribution function. The observation connecting the conic quadratic form of (5.2) and the probabilistic constraint (5.1) can however be stated more generally without empirical knowledge of the underlying distribution of $\boldsymbol{\xi}$. In particular, for $\mathbf{x} \in \{0,1\}^m$

$$\mathbb{P}\left(\boldsymbol{\xi}^\top \mathbf{x} \geq d\right) \geq 1-\epsilon \ \Rightarrow \ \mathbf{u}^\top \mathbf{x} - \Omega \parallel \boldsymbol{\Sigma}^{1/2} \mathbf{x} \parallel \geq d,$$

where $\Omega > 0$.

5.2 Problem Formulation

We will focus our attention to the conic quadratic restriction (5.2) of the probabilistic constraint (5.1) for the remaining analysis in the paper. In addition, we assume the coefficient of variation for each arc $e \in A$ is bounded (Ω as defined earlier).

$$\frac{\sigma_e}{u_e} \leq \frac{1}{\Omega}$$

We can formulate the following MIQCP, a robust formulation for network design with uncertain arc capacities (R-FCNF).

$$\begin{array}{lll} & \text{minimize} & \mathbf{f}^\top \mathbf{x} \\ \text{(R-FCNF)} & \text{subject to} & \mathbf{u}_C^\top \mathbf{x}_C - \Omega \parallel \boldsymbol{\Sigma}_C^{1/2} \mathbf{x}_C \parallel \geq d, \quad \forall\, C \in \mathcal{C} \\ & & \qquad \mathbf{x} \in \{0,1\}^m \end{array}$$

where $\mathbf{u}_C$ is vector of nominal values of arc capacities corresponding to the cut $C \in \mathcal{C}$ and $\boldsymbol{\Sigma}_C$ denotes the variance-covariance matrix of arc capacities corresponding to $C \in \mathcal{C}$, $\Omega > 0$.

It can be easily seen that (R-FCNF) is NP-hard as it generalizes (FCNF). The feasible set is obtained by intersection of exponentially many second order integer cone constraints. The following sections entail deriving fast solution procedures by analyzing the structure of the problem in context, first generally and subsequently with particular attention to independent and correlated nature of the arc capacities respectively.

5.3 Linearization of the Constraints

One of the main hurdles that makes solving non-linear integer problems computationally intractable is the need to solve non-linear continuous relaxations of these problems at each node of the branch and bound tree. Linearizations of the non-linear programs have proven to be effective [21, 93, 34]. The most common procedures to linearize a conic constraint entail either lift and project methods such as Reformulation Linearization Technique [85] or Outer Approximations [34, 21]. In the following, we contrast two such procedures relevant in the problem context.

5.3.1 McCormick Linearizations

Consider the conic quadratic constraint corresponding to $C \in \mathcal{C}$

$$\Omega\sqrt{\mathbf{x}_C^\top \boldsymbol{\Sigma}_C \mathbf{x}_C} \leq \mathbf{u}_C^\top \mathbf{x}_C - d \;\;\Leftrightarrow\;\; \left(\Omega^2 \left(\mathbf{x}_C^\top \boldsymbol{\Sigma}_C \mathbf{x}_C\right) \leq \left(\mathbf{u}_C^\top \mathbf{x}_C - d\right)^2\right) \cap \left(\mathbf{u}_C^\top \mathbf{x}_C \geq d\right)$$

We can linearize the above conic quadratic constraint using McCormick inequalities (1.8) in the following manner

$$\begin{aligned} \sum_{i \in C} \left(u_i^2 - \Omega^2 \sigma_i^2 - 2\, u_i d\right)\, x_i + 2 \sum_{i \in C} \sum_{\substack{j \in C \\ j > i}} \left(u_i u_j - \Omega^2 \sigma_{ij}\right) y_{ij} + d^2 \geq 0 \\ x_i + x_j \leq y_{ij} + 1 \quad \forall\, i, j \in C \\ y_{ij} \leq x_i \quad \forall\, i, j \in C \\ y_{ij} \leq x_j \quad \forall\, i, j \in C \\ x_i \in \{0, 1\} \quad \forall\, i \in C. \end{aligned}$$

It is worth a notice the aforementioned constraints implicitly restrict y_{ij} to be binary. A problem with the above linear constraints however is that instead of strengthening the feasible set they lead to a relaxation of the original problem more often than not. Besides further weakening the relaxation, the number of new variables incorporated in the above linearization is $O(|A|^2)$, which adds to another difficulty in the aforementioned formulation. Padberg [73] studied the convex hull of the boolean quadric polytope and further strengthened the relaxations arising from linearizations of bilinear terms. McCormick relaxations in particular and lift and project procedures suffer from a curse of dimensionality, growing quadratically in the lifted solution space. As we will see in the following, we can explore the structure of the problem in context to provide a computationally effective reformulation. In general solving large problems ($|V| \geq 50$) using this approach is rather inconceivable.

5.3.2 Supporting Hyperplane Relaxation

This linearization approach utilizes the gradient of the second order cone constraints to compute their outer approximation. Let the conic constraint obtained from the separation problem be $f(\mathbf{x}) \leq 0$. First order Taylor approximation of $f(\mathbf{x})$ around $\bar{\mathbf{x}}$ is given by

$$f(\mathbf{x}) = f(\bar{\mathbf{x}}) + (\mathbf{x} - \bar{\mathbf{x}})^\top \nabla f(\bar{\mathbf{x}}). \tag{5.3}$$

Since we are interested in a tangential approximation of the conic constraint, we need to choose $\bar{\mathbf{x}}$ on the surface $f(\mathbf{x}) = 0$, thus $f(\bar{\mathbf{x}}) = 0$, which implies

$$f(\mathbf{x}) = (\mathbf{x} - \bar{\mathbf{x}})^\top \nabla f(\bar{\mathbf{x}}). \tag{5.4}$$

We chose $\bar{\mathbf{x}}$ as the projection of the relaxation solution on the surface $f(\mathbf{x}) = 0$, i.e. point on the conic surface at the minimum (*euclidean*) distance from $\underline{\mathbf{x}}$ and use the gradient at that point to construct the supporting hyperplane. This choice of $\bar{\mathbf{x}}$, ensures the convergence of the algorithm. We incorporate the obtained linear constraint to obtain the new feasible set of the relaxation of (R-FCNF). In particular, we add the linearized constraint

$$\left(\mathbf{u} - \Omega \frac{\mathbf{\Sigma}\bar{\mathbf{x}}}{\sqrt{\bar{\mathbf{x}}^\top \mathbf{\Sigma}\, \bar{\mathbf{x}}}}\right)^\top (\mathbf{x} - \bar{\mathbf{x}}) \geq 0 \ . \tag{5.5}$$

Observe that while the hyperplane relaxation doesn't require incorporating additional variables in the formulation, one cannot provide bounds on number of hyperplanes required to represent the feasible set of (R-FCNF). Even though we cannot reduce the size of linearizations obtained using McCormick Inequalities, we can still strengthen the relaxations obtained by the supporting hyperplanes while preserving the dimensionality of the original solution space.

Although the linearizations discussed provide a way of eliminating the non-linearities in the formulation, they still do not provide an efficient procedure to solve (R-FCNF). Adding the additional variables leads to an explosion in terms of the number of variables for large problems, and the outer approximation whilst guaranteeing convergence, cannot ensure finiteness of the relaxation. Notice that since the network design problem in context involves only binary variables, the underlying feasible set of the problem is polyhedral. The following section discusses the polyhedral structure of the feasible regions in context of the aforementioned cases.

5.4 Strengthening the Formulation

The specific case when the arc capacities are independent warrants individual consideration as we can explore the specific combinatorial structure of the problem. We will thus discuss the two cases : independent capacities and correlated capacities, separately in Sections 5.4.1 and 5.4.2 respectively.

5.4.1 Independent Arc Capacities

In this section we address the case when the capacities on the given arcs although uncertain, are independent. In particular, we will consider the case when the variance covariance matrix $\mathbf{\Sigma}$ is diagonal. In this particular case the probabilistic constraint (5.1) can be modeled as the following conic quadratic 0-1 covering knapsack

$$X := \left\{ \mathbf{x} \in \{0,1\}^m \ : \ \mathbf{u}^\top \mathbf{x} - \Omega\sqrt{\boldsymbol{\sigma}^\top \mathbf{x}} \geq d \right\},$$

where $\boldsymbol{\sigma}$ is the vector of the variances $\boldsymbol{\sigma} := (\sigma_1^2, \sigma_2^2, \ldots, \sigma_m^2)$.

As observed in Chapter 2, conv(X) is a special case of a supermodular covering knapsack set. We will use the inequalities developed in Chapter 2 to strengthen the continuous relaxation of the master problem and thus improving solution times for the network design problem. The computational effectiveness of the pack inequalities and their extensions for the robust network design problem *vis-à-vis* CPLEX is highlighted in Section 5.6.

We lose this explicit combinatorial structure once the correlations are introduced in the robust network design problem, and in turn the valid inequalities derived thereof. In the following section we highlight how we can recover this combinatorial structure when taking into account the correlations amidst the arc capacities.

5.4.2 Correlated Arc Capacities

As observed in the earlier section, incorporating correlations into the robust network design problem voids the validity of pack inequalities and their extensions. Notice however, that the pack inequalities derived in Chapter 2 only require the underlying set function to be non-decreasing. Proposition 2.6 provides a sufficient condition that preserves the validity of pack inequalities in a special case when the covariance matrix $\mathbf{\Sigma}$ is not necessary diagonal. This sufficiency condition is often hard to satisfy and in general the pack inequalities and their extensions as discussed in Chapter 2 are not valid necessarily. While we cannot preserve the monotonicity of f, Chapter 3 provides a way to preserve the combinatorial structure of the set function in presence of correlations.

Define the set function $f_d : \{0,1\}^n \mapsto \mathbb{R}$ as

$$f_d := \sum_i \alpha_i x_i + 2 * \sum_i \sum_{j>i} \beta_{ij} x_i x_j + d^2, \tag{5.6}$$

where $\alpha_i = (\Omega^2\sigma_i^2 + 2u_i d - u_i^2)$ and $\beta_{ij} = (\Omega^2\sigma_{ij} - u_i u_j) \leq (\Omega^2\sigma_i\sigma_j - u_i u_j) \leq 0$. Observe the following equivalence with reference to the set functions f and f_d.

$$\{\mathbf{x} \in \{0,1\}^n\}\, f(\mathbf{x}) \geq d = \{\mathbf{x} \in \{0,1\}^n\}\, f_d(\mathbf{x}) \leq 0 \ \cap \ \mathbf{u}^\top \mathbf{x} \geq d. \tag{5.7}$$

While f is neither monotone nor submodular/supermodular, there are special properties and structure associated with f_d that can be explored to derive strong valid inequalities for the feasible set in consideration.

Corollary 5.1. *The set function $f_d(\mathbf{x})$ is submodular.*

This combinatorial characterization of the master problem yields a means to explore the polyhedral structure of the problem as discussed in Chapter 3. We present our computational analysis with the inequalities developed in Chapter 3 applied to the network design problem in Section 5.6.

5.5 Separation Problem

In Section 5.2 we presented the mathematical formulation for the robust network design problem and the studied the polyhedral structure of the constituting conic quadratic constraints. Besides being a computationally hard problem, (R-FCNF) incorporates exponential number of such conic quadratic constraints, since the number of s-t cuts in a connected graph is 2^{n-2}. Pertaining to this concern, we suggest an implicit formulation which incorporates a row generation method to determine solutions to (R-FCNF). For this formulation we require a separation oracle which either provides a violated conic constraint or a certificate of optimality for (R-FCNF). Given a feasible solution $\underline{\mathbf{x}}$, and the projections of $\mathbf{u}$ and $\mathbf{\Sigma}$ on $\underline{\mathbf{x}}$ as $\mathbf{u}_{\underline{\mathbf{x}}}$ and $\mathbf{\Sigma}_{\underline{\mathbf{x}}}$ to any relaxation of (R-FCNF) we can find a violated conic constraint using the following separation problem (SEP-$\underline{\mathbf{x}}$), formulated as the *robust minimum-cut problem.*

$$
\begin{array}{llrll}
 & \text{minimize} & \Theta(\underline{\mathbf{x}}) = & \mathbf{u}_{\underline{\mathbf{x}}}\mathbf{z} - \Omega\sqrt{\mathbf{z}^\top \mathbf{\Sigma}_{\underline{\mathbf{x}}}\mathbf{z}} & \\
(\text{SEP-}\underline{\mathbf{x}}) & \text{subject to} & \lambda_i - \lambda_j \leq & z_{ij} \quad (ij) \in A & (5.8)\\
 & & \lambda_i \geq & z_{ij} \quad (ij) \in A & (5.9)\\
 & & \lambda_j \leq & 1 - z_{ij} \quad (ij) \in A & (5.10)\\
 & & \lambda_s = & 1 & (5.11)\\
 & & \lambda_t = & 0 & (5.12)\\
 & & \lambda_i, \lambda_j \geq & 0 \quad (ij) \in A & (5.13)\\
 & & z_{ij} \in & \{0,1\} \quad (ij) \in A. & (5.14)
\end{array}
$$

Constraints (5.8), (5.9) and (5.10) ensure that only the arcs going from source set to sink set are included in the cut-set. Notice that for the deterministic minimum cut problem, only (5.8) is sufficient. Observe that (SEP-$\underline{\mathbf{x}}$) is NP-hard, since for $\mathbf{u} = \mathbf{0}$ and $\mathbf{\Sigma}$ diagonal, (SEP-$\underline{\mathbf{x}}$) reduces to the max-cut problem.

A close look at the separation problem reveals that unlike master problem the separation problem does not have a convex continuous relaxation which in turn renders this problem in the present form computationally intractable. Solving separation problem fast is of deep interest and importance to developing fast solution procedures for (R-FCNF). In the following sections we will explicitly discuss the two cases with reference to the separation problem, namely - independent capacities and correlated capacities. As we will demonstrate the two cases indeed require separate analyses because of completely different underlying polyhedral structure for the problem.

5.5.1 Independent Arc Capacities

In the particular case when the arc capacities are independent, the variance covariance matrix is diagonal and the separation problem for a relaxation solution $\underline{\mathbf{x}}$ can be formulated as following.

$$\begin{aligned} & \text{minimize} \quad \Theta(\underline{\mathbf{x}}) = \mathbf{u}_{\underline{\mathbf{x}}}^\top \mathbf{z} - \Omega \sqrt{\sum_{e \in A} \sigma_e^2 \underline{x}_e^2 \ z_e^2} \\ \text{(SEP-}\underline{\mathbf{x}}\text{)} \quad & \text{subject to} \quad (5.8) - (5.14). \end{aligned}$$

As observed earlier, (SEP-$\underline{\mathbf{x}}$) has a concave objective function $\Theta(\underline{\mathbf{x}})$. Utilizing the fact that $\Theta(\underline{\mathbf{x}})$ is a set function and, in particular, $\mathbf{z}$ is a binary vector, $\Theta(\underline{\mathbf{x}})$ can be equivalently expressed as

$$\Theta(\underline{\mathbf{x}}) = \mathbf{u}_{\underline{\mathbf{x}}}^\top \mathbf{z} - \Omega \sqrt{\sum_{e \in A} \sigma_e^2 \underline{x}_e^2 \ z_e} \quad . \tag{5.15}$$

The objective function $\Theta(\underline{\mathbf{x}})$ expressed as in (5.15) assumes the form (2.2) and hence is thus a non-decreasing supermodular set function. Minimizing a supermodular set function is a hard problem in general. Consider the following preliminaries with respect to the problem of minimizing a supermodular set function.

Proposition 5.1. [72] *If f is a supermodular set function on an index set N, then*

1. $f(T) \geq f(S) - \sum_{i \in S \setminus T} \rho_i(N \setminus i) + \sum_{i \in T \setminus S} \rho_i(S), \ \forall S, T \subseteq N;$
2. $f(T) \geq f(S) - \sum_{i \in S \setminus T} \rho_i(S \setminus i) + \sum_{i \in T \setminus S} \rho_i(\emptyset), \ \forall S, T \subseteq N.$

Proposition 5.1 implies that the either of the two inequalities

$$w \geq f(S) - \sum_{i \in S} \rho_i(N \setminus i)(i - x_i) + \sum_{i \in N \setminus S} \rho_i(S) x_i, \ \forall S \subseteq N \tag{5.16}$$

$$w \geq f(S) - \sum_{i \in S} \rho_i(S \setminus i)(i - x_i) + \sum_{i \in N \setminus S} \rho_i(\emptyset) x_i, \ \forall S \subseteq N \tag{5.17}$$

can be used to formulate the problem of minimizing supermodular f as a linear mixed 0-1 program [70]. Ahmed and Atamtürk [3] observed that for higher dimensions the linearizations using (5.16) or (5.17) aren't computationally effective.

Alternativerly, observe that $\Theta(\underline{\mathbf{x}})$ expressed as (5.15) is convex over $\mathbf{z} \in [0,1]^m$. The separation problem can thus be reformulated as the following convex quadratically constrained problem.

$$\begin{array}{lll} & \text{minimize} & \Theta(\underline{\mathbf{x}}) = \mathbf{u}_{\underline{\mathbf{x}}}^\top \mathbf{z} - t \\ (\text{SEP-}\underline{\mathbf{x}}\text{ - MIQP}) & \text{subject to} & t^2 \leq \Omega^2 \sum_{e \in A} \sigma_e^2 \underline{x}_e^2 \; z_e \\ & & (5.8) \; - \; (5.14). \end{array}$$

Solving the separation problem fast is imperative to the computational effectiveness of any algorithm to find an optimal solution of the robust network design problem. In the following we contrast the two methodologies discussed above to solve the separation problem in case of independent arc capacities namely, via the MIQP reformulation (SEP-$\underline{\mathbf{x}}$-MIQCP) and via the linearization obtained using (5.16) and (5.17). We use the MIP solver of CPLEX version 12.6 on a 2.93GHz Pentium Linux workstation with 8GB main memory.

Table 5.1: Separation problem : MIQP vs supermodular linearizations

nodes	arcs	Ω	MIQP		Inequalities (5.16)-(5.17)	
			nodes	time	nodes	time
50	1225	1	0	0.4	15	0.9
		3	0	0.4	18	1.1
		5	0	0.4	21	1.5
70	2415	1	0	1.4	12	3.2
		3	0	1.4	17	4.4
		5	0	1.4	30	6.4
100	4950	1	0	5.3	14	16.9
		3	0	5.6	25	20.3
		5	0	5.6	41	26.6

Table 5.1 contrasts the computational performance of the two approaches. The results tabulated are averaged over 5 randomly generated instances. The first column lists the number of nodes, the second column tabulates the number of arcs. The following columns depict the scaling factor Ω, number of nodes explored and times to optimal solutions for MIQP reformulation and linearization respectively. We observed that the convex quadratic reformulation of the separation problem can be solved manyfold faster. We will utilize this reformulation to solve the separation problem during our computational analysis in the case of independent capacities.

5.5.2 Correlated Arc Capacities

Amongst various other issues, the dependence of the arc capacities primarily affects the solution times for the separation problem (SEP-$\underline{\mathbf{x}}$). From a computational perspective the problem of network design with stochastic correlated arc capacities is prohibitive as such. This can be attributed to the non-convexities in the continuous relaxation of the feasible set of the separation problem resulting from the bilinear terms involved in the constraint set.

Although we have a convexification/linearization procedures to address the non-convexities arising due to bilinear terms as discussed in Section 5.3, these reformulations fail to address large problems. An alternative approach to address this issue can be devising a reformulation without lifting the feasible set into higher dimensions. In particular, we reformulate the separation problem with correlations as a MIQCP using a similar set function as in Section 5.4.2. In the following we devise a reformulation for the separation problem as a quadratically constrained program.

To introduce the idea of a MIQCP reformulation, we will first introduce the nesting of three sets corresponding to feasible solutions of

a) all possible network configurations, $\mathcal{A}$,

b) network configurations which satisfy the demand d nominally, $\mathcal{A}_n$, and

c) network configurations that satisfy the demand d in a robust manner $\mathcal{A}_r$.

Observe that $\mathcal{A}_r \subseteq \mathcal{A}_n \subseteq \mathcal{A}$. $\mathcal{A}_n$ can be obtained by separating minimum cuts with cut capacities satisfying the demand d. In this case, the separation problem reduces to the deterministic minimum cut problem which can be solved efficiently. To reduce $\mathcal{A}_n$ to $\mathcal{A}_r$ we solve the following MIQCP for $d' = d - \epsilon$, and sufficiently small $\epsilon > 0$.

$$\begin{array}{lll} & \text{minimize} & \Theta(\underline{\mathbf{x}}) = \mathbf{u}_{\underline{\mathbf{x}}}^\top \mathbf{z} \\ (\text{SEP-}\underline{\mathbf{x}}\text{-MIQCP}) & \text{subject to} & (\mathbf{u}_{\underline{\mathbf{x}}}^\top \mathbf{z} - d')^2 \leq \Omega^2 \cdot \mathbf{z}^\top \mathbf{\Sigma}_{\underline{\mathbf{x}}} \mathbf{z} \\ & & (5.8) - (5.14). \end{array} \tag{5.18}$$

Any feasible solution to (SEP-$\underline{\mathbf{x}}$-MIQCP) yields a violated conic constraint for the master problem. Infeasibility of (SEP-$\underline{\mathbf{x}}$-MIQCP) on the other hand serves as the certificate of optimality for the solution $\underline{\mathbf{x}}$. We summarize the algorithm to solve the separation problem with correlations as below.

Algorithm 2 Algorithm to solve Separation Problem with Correlations

1: **Input** Present incumbent solution from the master problem $\underline{\mathbf{x}}$

2: **Output** Violated Cut C

3: Solve the deterministic minimum cut problem with the incidence vector $\underline{\mathbf{x}}$.

4: If the nominal minimum cut capacity $< d$, add the minimum cut constraint to the master problem. Else go to next step (for all subsequent relaxation solutions).

5: Add the convex quadratic constraint $f_{d'}(\mathbf{x}) \leq 0$ and resolve the separation problem.

6: If the separation problem is infeasible, $\underline{\mathbf{x}}$ is optimal network configuration. Else **return** violated cut C.

Observe that with $f_{d'}$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ as defined in (5.6), constraint (5.18) can be equivalently stated as

$$f_{d'}(\mathbf{x}) \geq 0 \Leftrightarrow \sum_i \alpha_i x_i + 2 * \sum_i \sum_{j>i} \beta_{ij} x_i x_j + d'^2 \geq 0, \tag{5.19}$$

In addition, since $\boldsymbol{\beta} \leq 0$, constraint (5.19) is convex over $\mathbf{x} \in [0,1]^n$. Solvers such as CPLEX cannot explore this particular observation, however CPLEX can handle pure $0-1$ quadratic constraints very effectively using a combination of linearizations and cutting planes.

In the following, we tabulate the times to first feasible and optimal solution for two different solution approaches that we have seen in this section, namely the McCormick relaxation and the $0-1$ quadratic reformulation. The results tabulated are averaged over 5 randomly generated instances. The first column lists the number of nodes, the second column tabulates the number of arcs. The following columns depict the scaling factor Ω, and times to first feasible and optimal solutions for McCormick relaxation and MIQCP reformulation respectively.

It is evident from the computations listed in Table 5.2 that the MIQCP reformulation provide much better computational performance with respect to the McCormick Linearizations. This is also of significance because the separation problem is called several times from the master problem and the smaller solution times can lead to high impact in the overall solution times for the robust network design problem with correlations.

5.6 Computations

In this section we present our computational experiments for testing the effectiveness the inequalities for solving the network design problems with probabilistic capacities. For the computational experiments we use the MIP solver of CPLEX* (version 12.6) that solves conic

*CPLEX is a registered trademark of IBM ILOG

Table 5.2: Separation problem : McCormick vs MIQCP (times in seconds.)

nodes	arcs	Ω	McCormick		MIQCP	
			feasible	optimal	feasible	optimal
20	105	1	4	4	0.05	0
		3	5	5	0.08	0.1
		5	5	6	0.07	0.1
30	231	1	80	100	0.5	0.5
		3	105	137	0.4	0.6
		5	105	201	0.6	9
40	432	1	1062	1242	6	19
		3	1342	1440	6	12
		5	1620	1857	7	18

quadratic relaxations at the nodes of the branch-and-bound tree. CPLEX heuristics are turned off, and a single thread is used. When comparing to default CPLEX, the MIP search strategy is set to traditional branch-and-bound, rather than the default dynamic search as it is not possible to add users cuts in CPLEX while retaining the dynamic search strategy. Owing to significantly different solution procedures, we have addressed both the master problem and the separation problem in the context of independent and correlated capacities individually. The solver time limits and memory limits have been appropriately adjusted to represent the difficulty of the problem instances. In case of the independent capacities the time limit and the memory limits are set to 1800 secs. and 500 MB respectively, whereas in the case of correlations, the respective numbers are 3600 secs. and 1 GB. All experiments are performed on a 2.93GHz Pentium Linux workstation with 8GB main memory.

We contrast the computational performance of various algorithms discussed in Section 5.2 to find optimal solutions to the robust network design problem. We utilize the appropriate solution procedures for the separation problem in the context of independent and correlated capacities as discussed in the previous section. Apart from the trivial performance indices i.e. time to optimality and the number of nodes explored in the branch and bound tree, we also contrast various algorithmic approaches with respect to the distance from optimality. Since we have employed a row generation approach one such measure can be the incumbent gap (zgap) which we define as the percentage difference between the objective value of the best solution found by the algorithm and the optimal objective value. However as observed particularly during the computational analysis in the case of independent arc capacities is that while in majority of cases, the best solution found by CPLEX is indeed the optimal solution, CPLEX is not able to prove optimality in the prescribed time limit. Thus in the case of the independent arc capacities we observe the root relaxation gap (rgap) defined as the percentage difference in the optimal objective value of R-FCNF and objective value at the root node of the branch and bound tree after all the requisite conic quadratic constraints have been added (i.e. if the present incumbent solution cannot be separated).

In Tables 5.3 and 5.4 we report the results of the computational experiments for independent and correlated capacities respectively. The performance draws a comparison for varying number of nodes in the graph(n), arcs (a), values for Ω, and the ratio of the demand to the maximum flow possible in the network with the required value of Ω (β). For each combination, five random networks are generated with mean arc capacities from uniform $[0, 100]$ and σ_i from uniform $\left[0, \frac{u_i}{\Omega}\right]$. The demand $d = \beta \cdot \varphi$, where φ = maximum flow possible through the network for the given value of Ω. So that network is not completely dense, we set the probability of having an arc $i \rightarrow j$ $(i, j \in N, i < j)$ between any two nodes as $\frac{100}{\sqrt{n}}$, while ensuring the connectedness of the network.

5.6.1 Independent Arc Capacities

In Table 5.3 we compare the root relaxation gap (*rgap*) of the conic quadratic relaxation as discussed, the numbers of cuts generated (*cuts*), the number of nodes explored *(nodes)*, the CPU time in seconds (*time*) and the number of instances solved to optimality (#) with several cut generation options. The value of the rgap is computed as $\frac{(f_r - f^*)}{f^*}$, where f_r denotes the objective value at the root node and f^* denotes the optimal objective. If none of the algorithms solve a given instance to optimality within the given time limit of 1800 secs, then f^* is the objective value of the best found solution across all algorithms. The columns under heading CPLEX show the performance of CPLEX with conic cuts added to the formulation. The other columns show the performance when linearized tangent cuts, and extended pack cuts are added respectively. The cuts are generated throughout the branch and bound tree using the respective algorithms for linearization and pack separation and extension as proposed in Chapter 2.

The observations in Table 5.3 establish the computational effectiveness of the extended pack inequalities in the context of robust network design problem. In addition to this expected behavior, one can observe that while the outer approximations native to CPLEX are faster on average, the root gaps corresponding to the linearizations described in Section 5.2 are relatively smaller. This can be attributed to the fact that these linearizations utilize problem information as opposed to the generic outer approximation schema of CPLEX.

Table 5.3: Comparison between effectiveness of adding supporting hyperplanes vs extended pack inequalities

				Conic Cuts					Cplex Outer Approximation					Supporting Hyperplane Approximation					Extended Packs				
nodes	arcs	β	Ω	rgap	cuts	nodes	time	#	rgap	cuts	nodes	time	#	rgap	cuts	nodes	time	#	rgap	cuts	nodes	time	#
			1	66.22	3	123	1	5	66.22	3	82	1	5	60.42	87	24	76	5	0	7	0	4	5
		0.3	3	68.48	7	394	1	5	068.48	7	226	3	5	64.9	89	21	71	5	12.03	11	1	6	5
			5	60.35	4	349	1	5	60.35	4	163	2	5	53.36	106	19	80	5	1.33	9	0	3	5
			1	54.35	5	264	1	5	48.95	5	158	0	5	46.39	77	20	62	5	20.49	9	1	5	5
10	18	0.5	3	59.68	6	408	3	5	59.68	6	161	4	5	51.49	66	19	60	5	0.19	11	0	6	5
			5	44	8	1817	8	5	44	8	1187	2	5	38.99	125	31	94	5	2.31	10	1	7	5
			1	42.21	6	386	1	5	40.93	6	278	2	5	38.85	82	18	68	5	3.02	11	1	4	5
		0.7	3	38.98	3	394	1	5	41.38	3	206	0	5	32.58	134	27	101	5	9.58	9	3	3	5
			5	56.86	11	1251	6	5	53.07	11	876	5	5	52.27	113	23	88	5	0.83	12	1	4	5
			1	70.78	21	28146	628	4	68.69	34	16424	16	5	60.86	836	81	398	5	7.98	102	6	8	5
		0.3	3	68.5	27	19620	591	5	68.5	29	3570	5	5	61.87	562	61	285	5	1.52	46	2	12	5
			5	67.31	23	19950	773	3	67.17	28	3236	6	5	51.63	469	42	237	5	7.18	60	3	12	5
			1	56.45	16	17876	639	4	52.01	32	22242	26	5	44.25	815	97	368	5	9.23	164	13	36	5
20	54	0.5	3	61.14	26	29287	887	3	56.93	53	51336	54	5	53.07	763	93	315	5	11.05	141	17	20	5
			5	59.54	22	21371	760	4	56.03	40	25241	25	5	50.49	1124	120	490	5	13.26	298	30	28	5
			1	51.79	21	38152	769	3	47.49	43	49404	49	5	41.67	801	122	416	5	8.67	150	13	27	5
		0.7	3	51.39	24	33386	761	4	46.66	36	32124	22	5	45.11	673	102	326	5	7.62	125	12	26	5
			5	51.3	22	53640	762	3	44.63	46	47598	40	5	38.18	579	93	300	5	9.32	80	6	10	5
			1	64.73	18	46877	1450	2	58.63	122	297893	624	4	41.99	2558	127	1729	1	14.5	819	46	66	5
		0.3	3	66.57	17	46226	1440	2	60.27	162	457997	936	3	48.27	1938	119	1323	2	14.75	1230	69	97	5
			5	68.28	16	49432	1473	1	59.68	138	586878	1118	2	52.38	2391	124	1629	1	21.65	737	47	53	5
			1	58.68	18	87071	1800	1	48.1	142	898215	1222	4	37.78	2526	138	1602	2	20.49	1458	89	131	5
40	153	0.5	3	62.27	17	82869	1800	1	54.51	179	1008149	1603	3	44.71	2608	143	1740	1	27.91	1485	169	177	5
			5	61.24	16	59570	1800	0	51.26	178	906390	1581	2	41.87	2845	189	1946	1	24.38	2155	247	424	4
			1	52.63	16	64761	1800	2	42.17	148	806376	1184	4	36.19	2378	129	1639	1	27.12	2357	227	428	4
		0.7	3	57.75	16	69720	1800	1	42.65	121	998075	1125	3	35.64	2169	121	1398	2	26.44	2304	204	436	4
			5	55.7	15	83062	1800	0	45.07	152	772617	1023	3	35.31	2281	175	1515	3	24.9	2201	254	432	4
			Average	58.41		31719	806		53.83		258782	396		46.69		84	670		12.14		54	91	
			Deviation	8.15					8.97					8.78					8.94				

5.6.2 Correlated Arc Capacities

In Table 5.4 we compare the incumbent gap (*zgap*) of the algorithms, the numbers of cuts generated (*cuts*), the number of nodes explored *(nodes)*, the CPU time in seconds (*time*) and the number of instances solved to optimality (#) with several cut generation options. The value of the zgap is computed as $\dfrac{(f_i^* - f^*)}{f^*}$, where f_i^* denotes the objective value the best solution found and f^* denotes the optimal objective. For an algorithm which solves the problem to optimality $f_i^* = f^*$. If no algorithms solves a given instance to optimality within the given time limit of 3600 secs, then f^* is the objective value of the best found solution across all algorithms. The columns under heading CPLEX show the performance of CPLEX with conic cuts added to the formulation. The other columns show the performance when cplex linearizations, extended polymatroid cuts, and aggregated cover cuts are added respectively. The cuts are generated throughout the branch and bound tree using the respective algorithms for linearization and cut generation as discussed in Section 5.4.2.

Table 5.4 distinctly establishes the effectiveness of the linearization obtained via extended polymatroid inequalities. Again, the linearization in this context utilize the problem structure and hence are particularly efficient *vis-à-vis* CPLEX outer approximation. The computational performance is further improved by strengthening the linearization via aggregated cover inequalities.

Table 5.4: Comparison of computational effectiveness: Cplex vs. extended polymatroid inequalities with aggregated covers

				CPLEX					CPLEX Outer Approximation					Extended Polymatroids					Extended Polymatroids with Aggregated Covers					
nodes	arcs	β	Ω	zgap	cuts	nodes	time	#	zgap	cuts	nodes	time	#	zgap	cuts	nodes	time	#	zgap	cuts	covers	nodes	time	#
			1	0	6	474	2.2	5	0	6	232	0.09	5	0	18	67	0.1	5	0	16	9	33	0.08	5
		0.3	3	0	6	675	3.44	5	0	5	280	0.1	5	0	16	71	0.05	5	0	14	10	27	0.07	5
			5	0	4	616	1.73	5	0	4	202	0.06	5	0	33	89	0.07	5	0	20	9	37	0.08	5
			1	0	7	468	2.56	5	0	7	314	0.11	5	0	43	104	0.11	5	0	39	17	58	0.12	5
10	21	0.5	3	0	7	1314	5.45	5	0	7	430	0.11	5	0	30	119	0.26	5	0	30	16	62	0.12	5
			5	0	8	901	10.54	5	0	8	427	0.17	5	0	54	174	0.16	5	0	39	21	70	0.17	5
			1	0	7	1523	7.56	5	0	7	721	0.19	5	0	44	190	0.22	5	0	56	25	84	0.2	5
		0.7	3	0	11	2670	20.42	5	0	11	855	0.33	5	0	53	204	0.37	5	0	52	26	98	0.23	5
			5	0	12	5614	97.78	5	0	12	2125	0.76	5	0	98	359	0.3	5	0	101	42	141	0.18	5
			1	24.02	29	25429	1327.86	4	0	11	5671	3.48	5	0	279	1834	1.29	5	0	208	141	248	0.78	5
		0.3	3	0	16	7690	238.65	5	0	16	3837	2.15	5	0	164	792	0.71	5	0	154	121	256	0.62	5
			5	0	10	4283	81.54	5	0	10	2784	1.17	5	0	118	395	0.52	5	0	90	62	155	0.41	5
			1	9.89	51	59031	2176.39	2	0	29	41528	33.71	5	0	423	4758	3.22	5	0	466	200	1132	2.52	5
20	54	0.5	3	4.12	41	36523	1712.4	4	0	31	14067	8.43	5	0	418	1793	1.67	5	0	344	167	531	1.5	5
			5	6.6	84	34812	1583.48	3	11.18	50	129362	727.26	4	0	258	1074	0.98	5	0	190	120	310	0.76	5
			1	13.29	25	38103	1254.51	4	0	33	46481	32.49	5	0	719	8237	10.83	5	0	397	197	1270	2.64	5
		0.7	3	9.67	66	102159	3600.01	0	0	44	28176	19.6	5	0	352	2192	2.08	5	0	238	134	647	1.2	5
			5	14.89	48	47892	1698.66	4	0	38	24963	24.26	5	0	346	2658	1.87	5	0	393	224	828	2.39	5
			1	18.36	46	32337	2854.49	2	0	68	56284	171.38	5	0	231	2304	1.71	5	0	387	222	672	2.92	5
		0.3	3	23.13	54	28538	2586.19	2	0	108	137584	844.77	4	0	507	5620	5.19	5	0	397	246	814	3.21	5
			5	21.16	100	33951	2735.24	2	0	87	77529	385.8	5	0	305	2582	2.21	5	0	191	139	460	1.48	5
			1	18.82	90	109833	3600.01	0	3.99	106	541575	2219.5	3	0	1244	24314	24.19	5	0	937	566	2596	9.47	5
30	101	0.5	3	16.67	21	65734	2850.65	2	8.09	83	330311	1612.24	4	0	1297	14424	15.9	5	0	1155	721	2999	14.67	5
			5	12.3	40	133861	3600.01	0	0	98	262583	1123.59	5	0	963	5186	5.47	5	0	866	479	1242	6.33	5
			1	30.65	67	83056	3600.01	0	9.18	108	644090	2892.87	2	0	1790	51076	63.11	5	0	1686	962	4759	28.8	5
		0.7	3	10.78	63	90960	3600.01	0	22.41	63	540993	1811.78	3	0	1977	49073	81.85	5	0	2168	1118	3411	27	5
			5	13.46	83	76914	3600.01	0	6.09	91	314039	984.82	4	0	1175	13124	15.7	5	0	1379	630	2022	11.31	5
Average				16	37	37976	1587	84	9.6	42	118794	478	124	0	480	7141	9	135	0	445	245	925	4	135
Deviation				6.97					6.5					0					0					

Chapter 6

Conclusion

In the last four chapters, we proposed methodologies and strategies to solve binary conic-quadratic programs in a branch-and-cut framework and provided an application in form of robust network design. In this chapter, we conclude the dissertation by highlighting the important aspects of the work done and by describing some open problems and future research areas.

In Chapter 2, we studied the supermodular covering constraint set associated with the non-increasing set function. These type of constraint sets frequently arise in probabilistic threshold satisfaction problems. The classical supermodular formulation of such problems into 0-1 programming appears to be computationally ineffective due to its weak linear programming relaxation. In order to address this difficulty we derived valid inequalities for the supermodular covering set in context and investigated their separation, extensions and lifting. To strengthen the derived pack inequalities we proposed an extension algorithm that exploits the special structure of the particular supermodular function. We computed the sequence independent bounds on the lifting coefficients for the facets of the underlying polyhedral set. Furthermore, we presented a computational study on using the polyhedral results derived for solving 0-1 optimization problems over conic quadratic constraints with a branch-and-cut algorithm.

A major assumption throughout Chapter 2 was monotonicity of the underlying set function. In Chapter 3 we studied a generalization of the monotone submodular knapsack polytope by relaxing the monotonicity assumptions. We saw that the polyhedral analysis of the $0-1$ linear knapsack can be extended via extended polymatroids to the submodular knapsack polytope. In particular, we generalized the cover and pack inequalities, lifting approaches and presented easily computable extensions and sequence independent bounds on the lifting coefficients for the general submodular knapsack. We presented both a theoretical discussion as well as a computational analysis for the effectiveness of the inequalities on submodular quadratic and general $0-1$ quadratic knapsack sets.

During our computational analysis in Chapter 3 We observed that the submodular cover inequalities obtained via aggregation of extended polymatroid inequalities proved to be effective in strengthening the root relaxation for the problem instances even with a simple aggregation heuristic. More work needs to be done to formalize the discussion on aggregation of extended polymatroid inequalities. It is expected that utilizing good aggregation heuristics can further strengthen the relaxations and improve the solution times.

In Chapter 4 we changed our perspective from studying the combinatorial structures of $0-1$ conic-quadratic sets to understanding the geometry of the general $0-1$ quadratic sets. We provided convexification techniques for $0-1$ non-convex quadratic sets. We derived strengthening procedures for these reformulations and a theoretical insight for the containment of these convex quadratic sets. We also derived a new linearization procedure to strengthen the convex reformulation. These linearizations are a modified version of the McCormick linearizations with half the number of constraints.

In Chapter 5 we studied an application of the methodologies developed in this dissertation. We looked at the problem of designing network configurations that are robust with respect to the uncertainty of arc capacities. We formulated the problem using probabilistic guarantees and provided a sufficient deterministic formulation as a $0-1$ conic quadratic constrained optimization problem. We considered a row generation approach and formulated the separation problem as the robust minimum cut problem. We derived solution methodologies and reformulations in order to solve the separation problem fast especially in the case of correlations, which renders the separation problem computationally prohibitive. In addition, we derived solution approaches for the master problem in the aforementioned contexts while paying particular attention to the combinatorial structure of the problem. An extensive computational analysis established the effectiveness of utilizing these approaches *vis-à-vis* CPLEX.

The importance of solving combinatorial optimization problems fast is far evident. Probabilistic counterparts of these problems relax the assumptions about the deterministic nature of the parameters. The need to develop solution procedures and algorithms to solve these problems efficiently in today's context is imperative and has far ranging applications in many fields such as healthcare, computational biology, transport engineering, information theory, etc. In this dissertation we have developed solution methodologies that revolve around a central theme of addressing these problems.

Fast solutions procedures to the aforementioned questions will find their applications in plethora of real life problems entailing flow networks i.e. transportation networks (shortest path under uncertainty, maximum traffic flow under uncertainty), communication networks (optimizing data transfer over variable bandwidths), pipe line flows, etc. In addition, further interest lies in formulating probabilistic versions of combinatorial problems such as matching in bipartite graphs and assignment problems within this framework.

A related, but interesting problem is when some of the variables are allowed to be continuous. For example, an immediate extension to the network design problems with parametric uncertainties can be seen as flow problems in these networks. Within the framework of network configurations with parametric uncertainties, we can pose the following questions:

1. What is the maximum flow that can be sent through this network configuration?
2. How to optimally route a given flow across this network from the source node to the sink node with a given confidence level.

Fast solutions procedures to the aforementioned questions will find their applications in plethora of real life problems entailing flow networks i.e. transportation networks (shortest path under uncertainty, maximum traffic flow under uncertainty), communication networks (optimizing data transfer over variable bandwidths), pipe line flows, etc. In addition, further interest lies in formulating probabilistic versions of combinatorial problems such as matching in bipartite graphs and assignment problems within this framework. It is important to observe that unlike in the case of linear knapsack problem [6] where it is trivial to characterize the coefficients of continuous variables in the linear knapsack problem, in the conic-quadratic case, the convex hull of feasible solutions is no longer a polyhedron, and one requires nonlinear inequalities to describe the convex hull of feasible solutions, with the continuous variables playing a nontrivial part.

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